

PANDA

Powder Analysis for Neutron Diffraction Applications

User Manual



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Instruments: D20 | D1B | D2B | D16 | XtremeD

Neutron Diffraction Data Browser & Analysis Tool

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1. Introduction

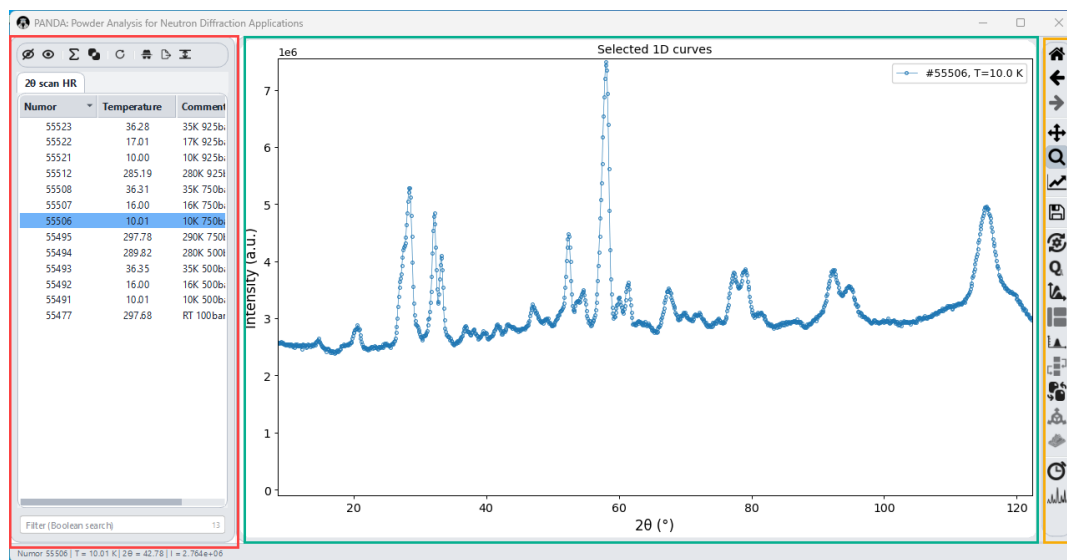
PANDA (Powder Analysis for Neutron Diffraction Applications) is a scientific data browser and analysis tool designed for neutron diffraction experiments. It allows researchers to load, visualize, combine, and analyze neutron diffraction datasets acquired at ILL instruments such as D20, D1B, XtremeD, D16 and D2B.

This manual describes all available features and how to use them effectively. It also includes instrument-specific guidance, scientific workflows, and best practices developed through real experimental use.

1.1 Main Interface Layout

The PANDA interface is divided into three main areas:

Area	Description
Left panel	File/numor browser with the dataset list and action toolbar
Center canvas	Main plot area for 1D patterns and 2D heatmaps
Right toolbar	Navigation and visualization tools (zoom, pan, export, etc.)



General layout of the PANDA graphical user interface. The interface is divided into three main regions: the left panel contains the file/numor browser together with the dataset list and action toolbar; the central area displays the main visualization canvas for 1D diffraction patterns and 2D heatmaps; and the right toolbar provides navigation and visualization tools, including zoom, pan and export functionalities.

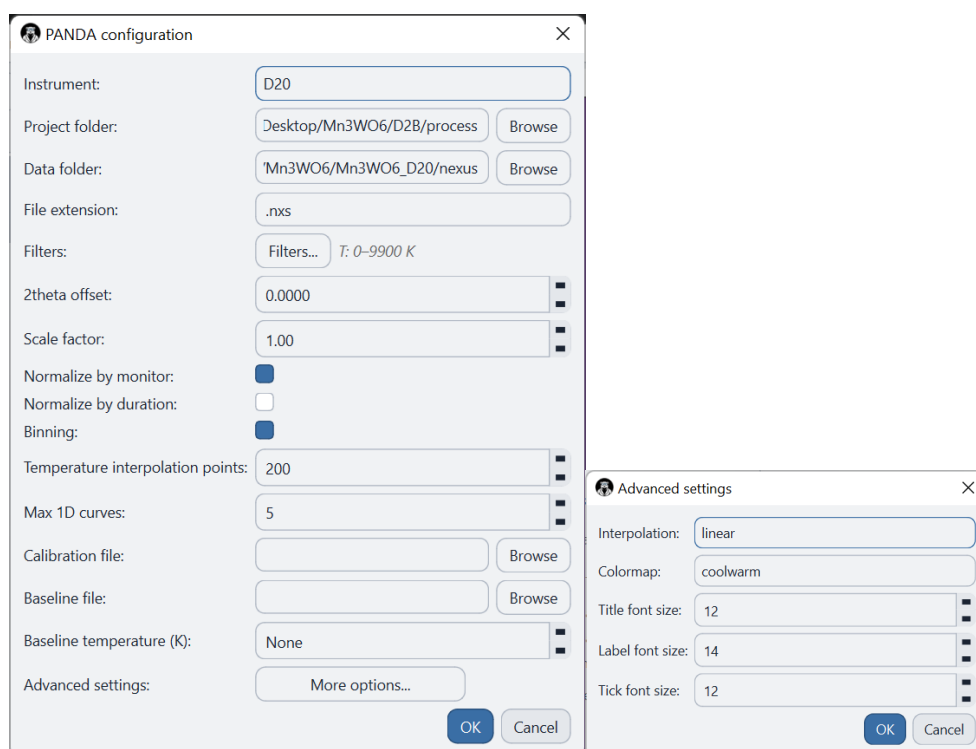
2. Configuration Window

The PANDA Configuration window is the entry point of the application. It appears at startup and can be reopened at any time via the Settings button in the right toolbar. All parameters are saved automatically to a

`user_config.py` file in the project folder and restored on the next launch.

NOTE: Changes take effect immediately after clicking OK. PANDA reloads the dataset list if instrument, folder, or filter settings change.

2.1 Field Reference



PANDA Configuration window showing the main setup parameters for a particular instrument, also accessible via the Advanced Settings button in the toolbar. Depending on the active instrument, some fields may differ. Fields include project and data folder paths, file extension filter, number and temperature ranges, angular correction, intensity scale factor, normalization mode, binning, heatmap interpolation points, maximum simultaneous 1D curves, and optional calibration and baseline files.

NOTE: The Advanced Settings dialog, accessible from the toolbar, allows fine-tuning of the visual parameters applied to all plot types. The available options are: Interpolation (controls the interpolation method used in 2D heatmap rendering, e.g. linear, nearest, bilinear), Colormap (sets the colour scale used in heatmap and 3D views, accepting any Matplotlib-compatible colormap name such as coolwarm, viridis, or plasma), and the font sizes for Title, Labels, and Ticks, which control the typographic scale of all plot annotations. Adjusting these parameters before export is recommended to produce figures that meet publication or presentation requirements without post-processing.

Field	Description
Instrument	Selects the ILL instrument that produced the data (e.g. D20, D2B, D1B or XtremD). Controls how NeXus files are parsed: axis labels, detector geometry, and available metadata fields all depend on this setting.
Project folder	Root folder of the experiment. PANDA saves user_config.py here. Typically the proposal folder on the ILL file system.
Data folder	Folder where the raw NeXus (.nxs) files are located. Can be the same as the project folder or a subdirectory. PANDA scans this folder for files matching the configured extension.
File extension	File type to scan for in the data folder. Default is .nxs (NeXus HDF5 format used by ILL instruments). Change only if data is stored with a non-standard extension.
Filters	Opens a sub-dialog to restrict which numors are loaded, filtering by: Temperature range (T min – T max, in K) and Numor range (N min – N max). Active filter summary shown inline, e.g. T: 0–500 K N: 286372–286495.
2θ offset	Rigid angular correction applied to all 2θ values (degrees). Corrects a systematic zero-point error in the detector position. $2\theta_{corrected} = 2\theta_{raw} + offset$. Default: 0.0000.
Scale factor	Global multiplicative factor applied to all intensities. Rescales raw counts or matches the scale expected by Rietveld refinement codes. Default: 1.00.
Normalize by monitor	Divides each dataset intensity by its monitor count before display, correcting for incident beam flux variations. The reference monitor is fixed at session start.
Normalize by duration	Divides intensities by the counting time (seconds). Useful when datasets in the same series have different acquisition durations.
Binning	Activates angular rebinning onto a regular 2θ grid. Required for combining or differencing datasets with slightly different native detector grids.
Temperature interpolation points	Number of Y-axis temperature points for the 2D heatmap. The temperature axis is interpolated onto this regular grid for a uniform image. Default: 200.
Max 1D curves	Maximum number of datasets displayed simultaneously in 1D overlay mode before automatically switching to the 2D heatmap. Default: 5.
Calibration file	Path to an instrument calibration file (e.g. .241 format for D20) that corrects for detector efficiency variations across the detector bank. Use Browse to navigate to the file.
Baseline file	Optional path to a reference NeXus pattern used as background baseline. When set, this pattern is subtracted automatically from all loaded datasets.
Baseline temperature (K)	Temperature of the baseline measurement in Kelvin, used to select the correct numor when the baseline file contains multiple temperatures. Set to None to disable.

IMPORTANT: All settings are persisted in user_config.py in the project folder and can also be edited manually with a text editor for batch configuration.

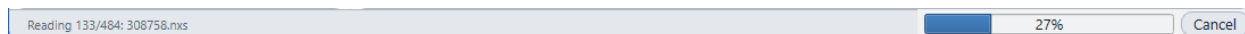
NOTE: If no NeXus files matching the selected extension are found in the configured Data folder, PANDA will display a dialog asking whether to Reconfigure or Cancel. Choosing Reconfigure allows the user to correct a possible mistake in the folder path or configuration settings. Choosing Cancel starts PANDA without loading any datasets.

NOTE: Most PANDA features are primarily designed to operate directly on NeXus files generated at the ILL. However, to increase the flexibility of the program, additional file formats are also supported, allowing exploratory analysis of datasets generated by third-party software or external instruments. At present, PANDA recognizes .xys and .dat files corresponding to column-based text formats, where the first column contains the diffraction coordinate (typically 2θ), the second column the intensities, and the last column the associated intensity errors. PANDA also includes support for the .xrdml format used by Malvern Panalytical instruments.

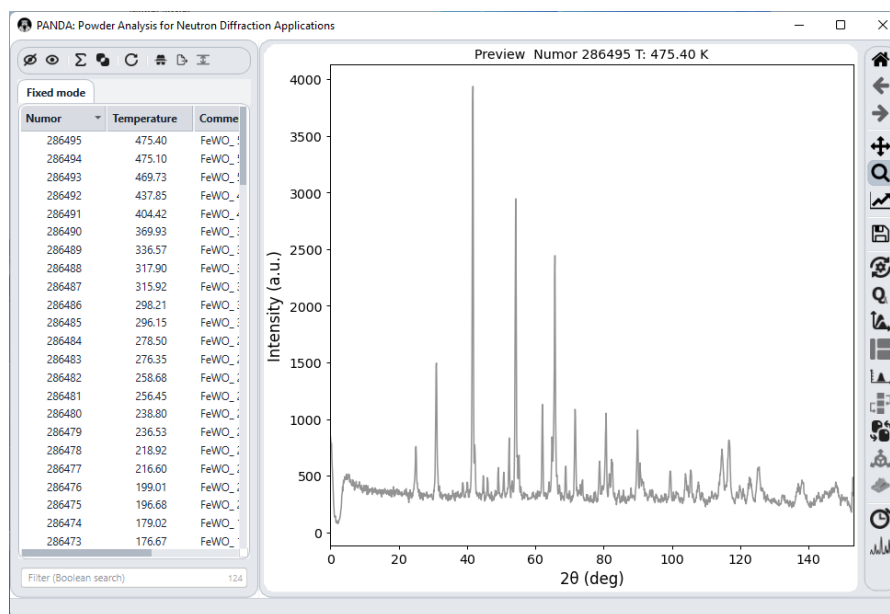
In addition, PANDA supports time-of-flight (TOF) powder diffraction data stored in GSAS .dat files compatible with the FullProf Instrument Parameter Set 12. Unlike conventional constant-wavelength diffraction data, these files contain diffraction patterns recorded as a function of neutron time-of-flight (TOF) rather than scattering angle. PANDA automatically recognizes the GSAS file structure, reads the TOF axis directly from the file header, and imports the associated intensity and statistical uncertainty values. This allows TOF datasets to be visualized, compared, and processed within PANDA in the same way as other supported diffraction formats. When the corresponding instrument calibration parameters (Dtt1, Dtt2, and optionally Zero) are available, PANDA can additionally convert the TOF scale into d-spacing and Q-space representations, facilitating direct comparison with data collected using other diffraction techniques and instruments. PANDA automatically searches file headers for temperatures and other relevant metadata whenever possible. Nevertheless, users can manually edit or complete the corresponding parameters directly in the dataset table when required.

3. Loading Data

PANDA automatically scans the configured data folder for NeXus (.nxs) files. All detected datasets are listed in the left panel organized by numor.



Status bar displayed during file loading. The progress indicator shows the number of Numors already loaded and the total number of files to be processed, allowing the user to monitor the loading progress, estimate the remaining time, and know how many Numors are still waiting to be loaded.



PANDA main interface showing a temperature series from a FeWO₄ sample measured on D20. The left panel lists 124 numors in Fixed mode (2θ was not moving during the measurements) with their numor number, temperature (K), and sample comment. The central canvas displays a hover preview of numor 286495 (475.40 K), showing the powder diffraction pattern (Intensity vs. 2θ) with the characteristic Bragg peaks of the high-temperature phase. The right toolbar provides access to navigation, zoom, export, and visualization tools

3.1 Automatic Loading

When launched, PANDA loads all NeXus files found in the configured data folder. Each file is parsed to extract:

- Numor (experiment number)
- Temperature (K)
- Comments / sample information
- Diffraction pattern (2θ axis and intensity)
- Monitor counts (for normalization)

3.2 Incremental Reload

Reload folder (Ctrl+R or toolbar button): re-scans the data folder and loads only new files since the last load. Essential during live experiments to pick up incoming numors without reloading everything.



The toolbar above the left panel provides the main dataset operations, including Reload Folder (fifth icon from the left), which re-scans the data folder and loads any new files incrementally.

TIP: Use Ctrl+R frequently during live measurements to monitor incoming data in real time.

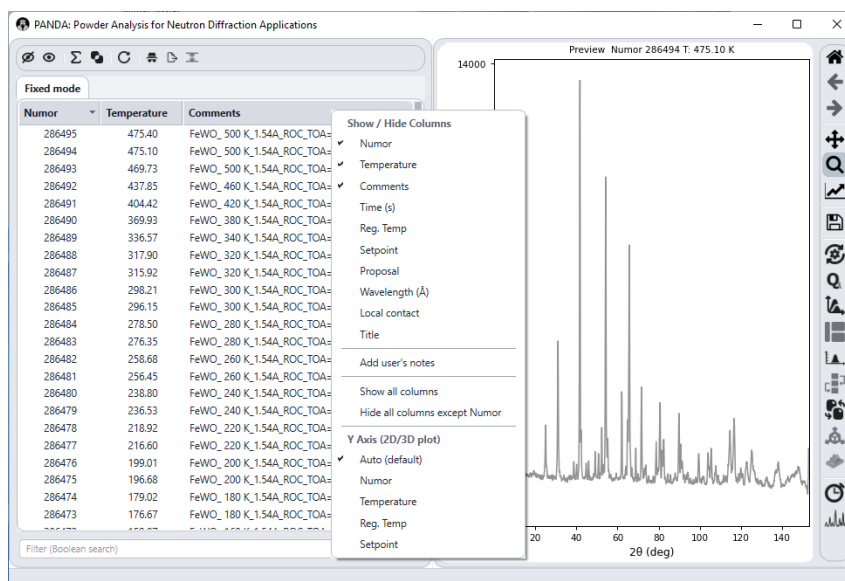
NOTE: The Reload Folder function is strictly incremental, it only adds new numors found in the data folder since the last load, and does not reset the current session state. Any numors that have been manually hidden will remain hidden after a reload; to make them visible again the user must explicitly use the Show All action (Ctrl+S). This behaviour is intentional, as it allows the user to maintain a curated view of the dataset list during a live experiment without losing their current selection or visibility settings.

3.3 Dataset Columns

Each row in the dataset list shows:

Column	Content
Numor	Unique experiment number assigned by the instrument control system
Temperature	Sample temperature in Kelvin at time of measurement
Comments	Free-text comment from the experiment log

The column widths are adjustable by dragging the column borders, allowing more content to be visible at once. A left-click on any column header sorts the list by that column, either numerically or alphabetically depending on the column type; clicking again reverses the sort order. A right-click on the column header opens a context menu to control which columns are displayed, making it possible to show or hide additional metadata fields available in the NeXus files.



Column visibility control in PANDA. Right-clicking on the column header opens the Show/Hide Columns context menu, which allows the user to toggle individual metadata fields (Numor, Temperature, Comments, Time, Reg. Temp, Setpoint, Proposal, Wavelength, Local contact, Title, and user notes). The menu also provides shortcuts to show all columns at once or hide all except Numor. The lower section of the menu controls the Y axis variable used in the 2D heatmap and 3D plots, with options including Auto (default), Numor, Temperature, Reg. Temp, and Setpoint.

IMPORTANT: The user can add specific comments to individual numors via the Add user's notes option in this menu. These comments are saved to the log file, ensuring that any relevant annotations are traceable and preserved as part of the experiment record.

NOTE: Table cells in PANDA are directly editable. To modify a value, either double-click on the corresponding cell or press the F2 key after selecting it. All fields can be edited except the numor column, which is always read-only.

Edited values are kept in memory during the active session and are automatically applied to all subsequent operations, including plotting, exporting, and dataset combination.

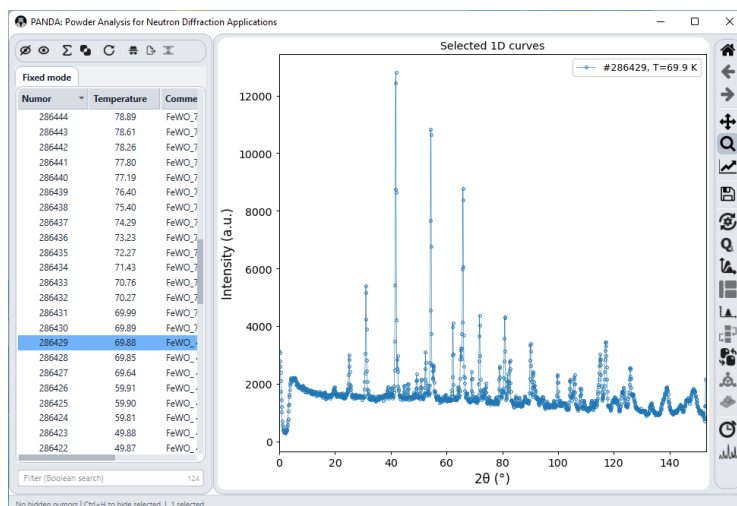
To ensure reproducibility and traceability of manual modifications, it is strongly recommended to save the corresponding log file containing the applied changes.

User edits are preserved when refreshing the trees, either by pressing Ctrl+R or by using the refresh action button.

NOTE: Column editing: PANDA also supports simultaneous editing of multiple rows within the same column. First, select a set of continuous rows in the tree view. Then place the cursor in the column to modify (for example, Wavelength), press F2, edit the value, and validate with Enter. The new value will automatically be applied to the selected column for all highlighted rows.

4. Visualization

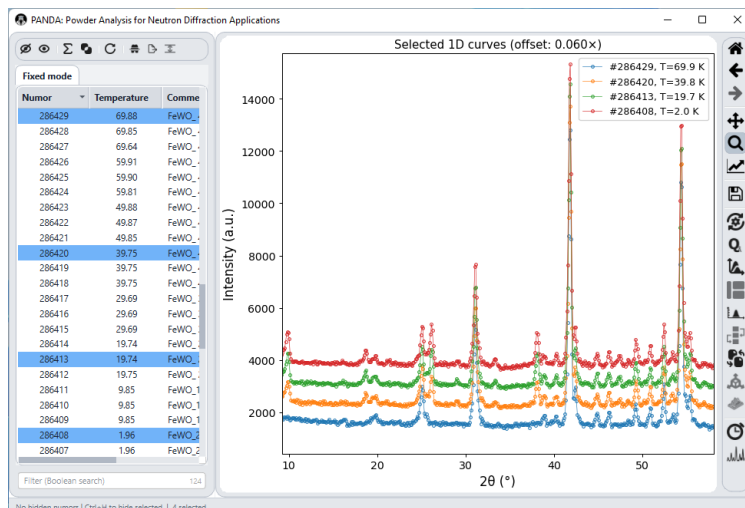
Selecting one or more datasets in the left panel immediately plots them in the central canvas. PANDA automatically adapts the plot type depending on the number of datasets selected. To deselect items, either right-click anywhere in the numor list area to clear the entire selection, or left-click on an already selected numor to deselect it individually.



PANDA main interface in 1D mode displaying a single selected diffraction pattern. The selected numor (286429, $T = 69.88$ K) is highlighted in blue in the dataset list and its corresponding powder diffraction pattern (Intensity vs. 2θ) is plotted in blue in the central canvas. The status bar at the bottom confirms the current state: no hidden numors, 1 dataset selected.

4.1 1D Mode — Diffraction Patterns

When one or a few datasets are selected, PANDA plots individual 1D diffraction patterns (Intensity vs. 2θ or Q). Multiple datasets are overlaid on the same axes for direct comparison.



PANDA main interface in 1D overlay mode with four datasets selected simultaneously (286429, 286420, 286413 and 286408, highlighted in blue in the dataset list), covering a temperature range from 2.0 K to 69.9 K. Each pattern is displayed in a distinct color matching its legend entry. A vertical offset between curves (offset: 0.060x, shown in the plot title) has been applied using the scroll wheel to separate the patterns along the Y axis for clarity. The zoom has been restricted to the 10–60° 2θ region of interest by clicking and dragging directly on the plot. The legend identifies each dataset by numor and temperature, providing immediate visual context for the comparison.

Available axes

- 2θ (degrees) — default angular axis
- Q ($\text{\AA}^{-1}$) — momentum transfer; toggle with the Q button in the toolbar

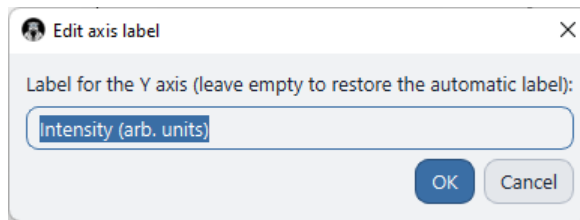
Log scale

Log button: switches the intensity (Y) axis between linear and logarithmic scale. Useful to inspect weak reflections alongside strong peaks.

4.2 2D Mode — Temperature Heatmap

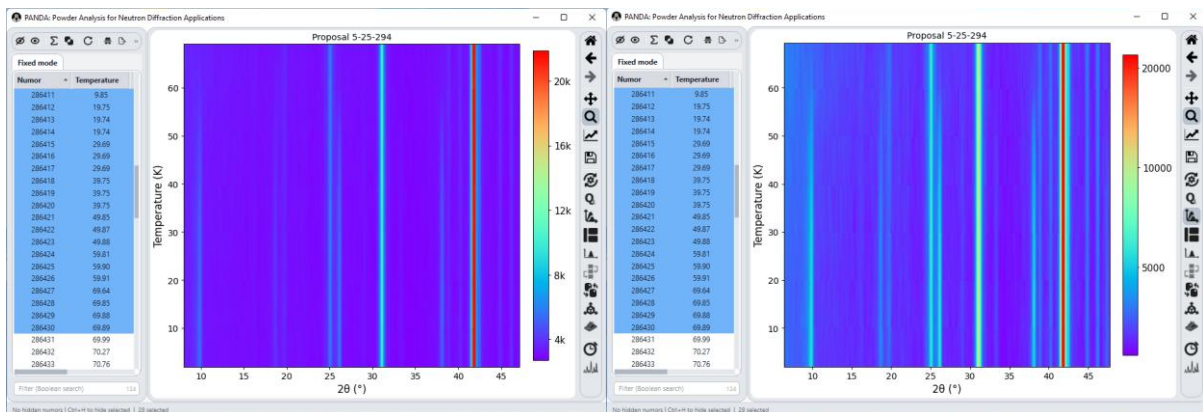
When many datasets are selected, PANDA automatically switches to a 2D heatmap where:

- X axis: 2θ or Q
- Y axis: temperature (or any other scan variable)
- Color: intensity (linear or logarithmic)



Double-clicking on any plot axis opens the axis label editor, allowing the user to define a custom label. The customized label is kept for the duration of the current session — restarting PANDA restores the automatic label. Special characters can be typed directly ($^{\circ}$, $\text{\AA}$) or inserted via the symbol picker (Win+.). Mathematical notation can be entered between $\$...\$$, rendered using Matplotlib syntax, e.g. Q ($\$AA^{\circ}\$$) $\rightarrow Q$ ($\text{\AA}^{-1}$), 2θ ($\$theta^{\circ}\$$) $\rightarrow 2\theta$ ($^{\circ}$), or $\$T_{\text{sample}}\$$ (K) for subscripts.

The heatmap gives an immediate overview of how the diffraction pattern evolves as a function of temperature, enabling rapid identification of phase transitions.



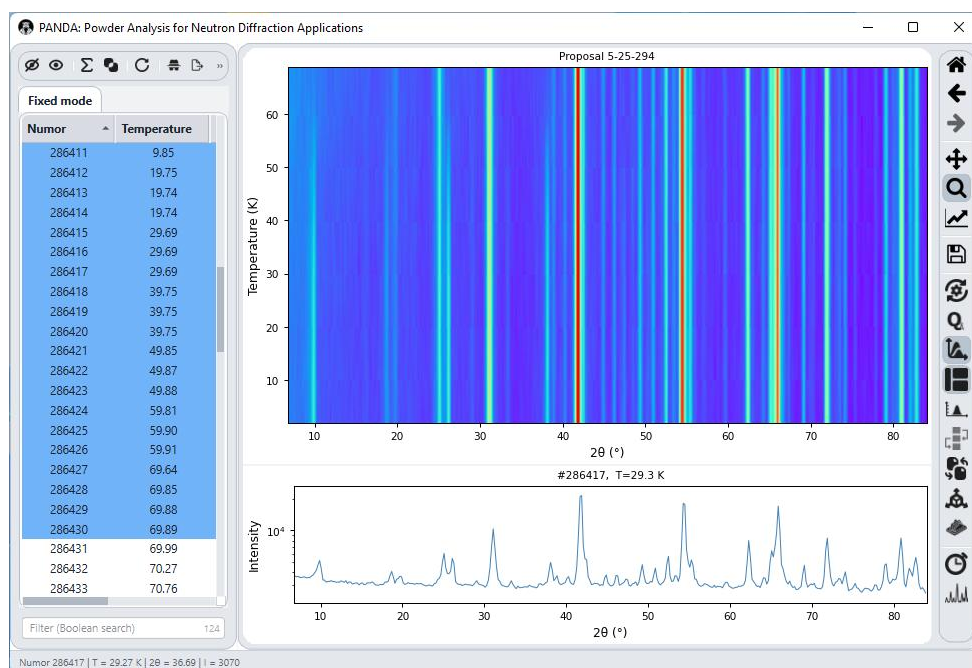
2D heatmap of the FeWO_4 temperature series (Proposal 5-25-294) with 28 numors selected, displaying diffraction intensity as a function of 2θ (x-axis) and temperature (y-axis, 9.85–69.89 K). The left panel shows the intensity on a linear color scale, where the strongest Bragg reflections near 42° dominate the color range and weaker features are barely visible. The right panel shows the same data on a logarithmic color scale, revealing weak reflections and subtle intensity changes across the full angular range that are hidden in the linear representation. Both panels share the same color bar range (0–20000 a.u.).

TIP: The color scale limits (minimum and maximum) as well as the color scheme can be adjusted via the Edit axis button in the right toolbar, identified by a zigzag arrow icon. This allows the user to fine-tune the intensity range and choose the most suitable color palette for the data, which is particularly useful for enhancing the contrast of weak features or suppressing the contribution of very intense peaks.

TIP: In the 2D heatmap mode, right-clicking outside the heatmap area opens a floating context menu that allows the user to hide or show the color bar. This is useful for maximizing the display area of the heatmap, for example when preparing figures for publication.

4.3 1D Slice Panel

Slice button: activates a secondary panel below the heatmap showing a horizontal slice (1D pattern) for the row under the mouse cursor. The slice updates in real time as you hover over the heatmap. The split between heatmap and slice panel is adjustable.



PANDA interface in 2D heatmap mode with the Slice panel activated (Proposal 5-25-294). The upper panel displays the full temperature-dependent heatmap (9.85–69.89 K), while the lower panel shows in real time the 1D diffraction pattern corresponding to the numor under the mouse cursor (numor 286417, $T = 29.3$ K), with the intensity axis in logarithmic scale. The status bar at the bottom confirms the current cursor position ($T = 29.27$ K, $2\theta = 36.69^\circ$, $I = 3070$). The relative size of the heatmap and slice panels can be adjusted freely by clicking and dragging the divider between them. The slice display can be combined with logarithmic intensity scaling or switched to the Q representation for instrument-independent comparison.

NOTE: Double-clicking on any 2D map activates a movable guide line that follows the mouse cursor. This feature can be useful as a visual reference when inspecting specific regions or tracking features across the map.

4.4 3D Views

PANDA provides two interactive 3D visualization modes that render the active 2D heatmap as a three-dimensional scene. Both views inherit the current heatmap state, zoom range, colormap,

intensity scale, and axis configuration, and are intended for visual inspection only; the underlying dataset is never modified. The horizontal axis reflects whichever space is active (2θ , Q , or TOF), the vertical axis corresponds to the configured metadata field (typically temperature), and height and colour both encode diffraction intensity. When logarithmic scale is enabled, height represents $\log_{10}(\text{Intensity})$.

View	Description	Recommended use
3D Surface	GPU-accelerated continuous surface with a waterfall line overlay (OpenGL)	Identifying intensity maxima, broad trends, and peak evolution across the vertical axis. Fast option.
3D Waterfall	Combined surface and stacked 1D profiles along the vertical axis	Similar to the previous but better image exportation for final reports.

Opening a 3D view

1. Select more than five compatible datasets (the minimum number can be configured in the initial settings window) to activate the standard 2D heatmap. The 3D toolbar buttons are enabled only while a heatmap is displayed.
2. Optionally, zoom into the heatmap region of interest before opening the 3D view. The 3D scene will use the visible region only, so pre-zooming is an efficient way to focus on a specific angular or Q range.
3. Click Open 3D visualization for the surface view, or 3D waterfall for the waterfall view.
4. To switch between the two 3D views, or to return to the 2D heatmap, simply click any dataset (numor) in the left-hand panel. PANDA will automatically restore the heatmap view, allowing a different 3D visualization to be opened if required.

3D Surface controls

The surface is rendered in a dedicated window. The following interactions and controls are available:

- *Rotate* - drag with the left mouse button.
- *Zoom* - scroll the mouse wheel.
- *Pan* - drag with the middle mouse button.
- *X / Y / Z sliders* - adjust the visual proportions of the plot along each axis. These affect the display only and do not modify the data.
- *W. Decim.* - controls the density of the waterfall line overlay. Higher values show fewer profiles; at the maximum value the overlay is hidden entirely.
- *Show axis* - toggles axis lines, tick values, and labels.

A colorbar on the right indicates the intensity scale. If the required 3D rendering support is unavailable on the system, PANDA displays a warning message instead of opening the view.

3D Waterfall controls

The waterfall view combines a coloured surface with stacked 1D diffraction profiles distributed along the vertical axis. Each profile preserves the full horizontal-axis resolution.

- *X / Y / Z sliders* - adjust the visual proportions of the plot.
- *W. Decim.* - reduces the number of displayed profiles by sampling along the vertical axis, improving readability and responsiveness without affecting the underlying data.
- *Show/hide surface* - toggles the coloured surface on and off.
- *Show/hide waterfall* - toggles the stacked profile lines on and off.

While rotating the view, PANDA temporarily uses a lighter rendering mode and restores full quality when the interaction ends. A colorbar indicates the intensity scale.

TIPS:

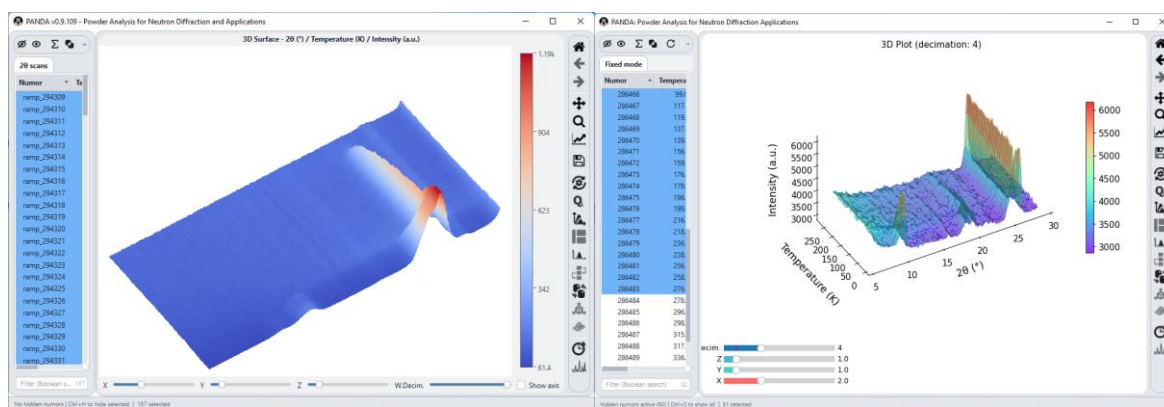
The Zoom the 2D heatmap to a region of interest before opening either 3D view to limit the rendered data to the range that matters, which also improves performance with large datasets.

Use the 3D Surface view for an overview of the intensity landscape and to locate anomalies or phase boundaries.

Use the 3D Waterfall view when individual profile shapes are important, such as when tracking a peak shift or monitoring the growth of a new reflection.

The X, Y, and Z sliders are useful for correcting aspect ratio distortions that arise when the horizontal and vertical axes cover very different numeric ranges.

To switch between the two views, close the 3D window first and re-enable the heatmap before clicking the other toolbar button.



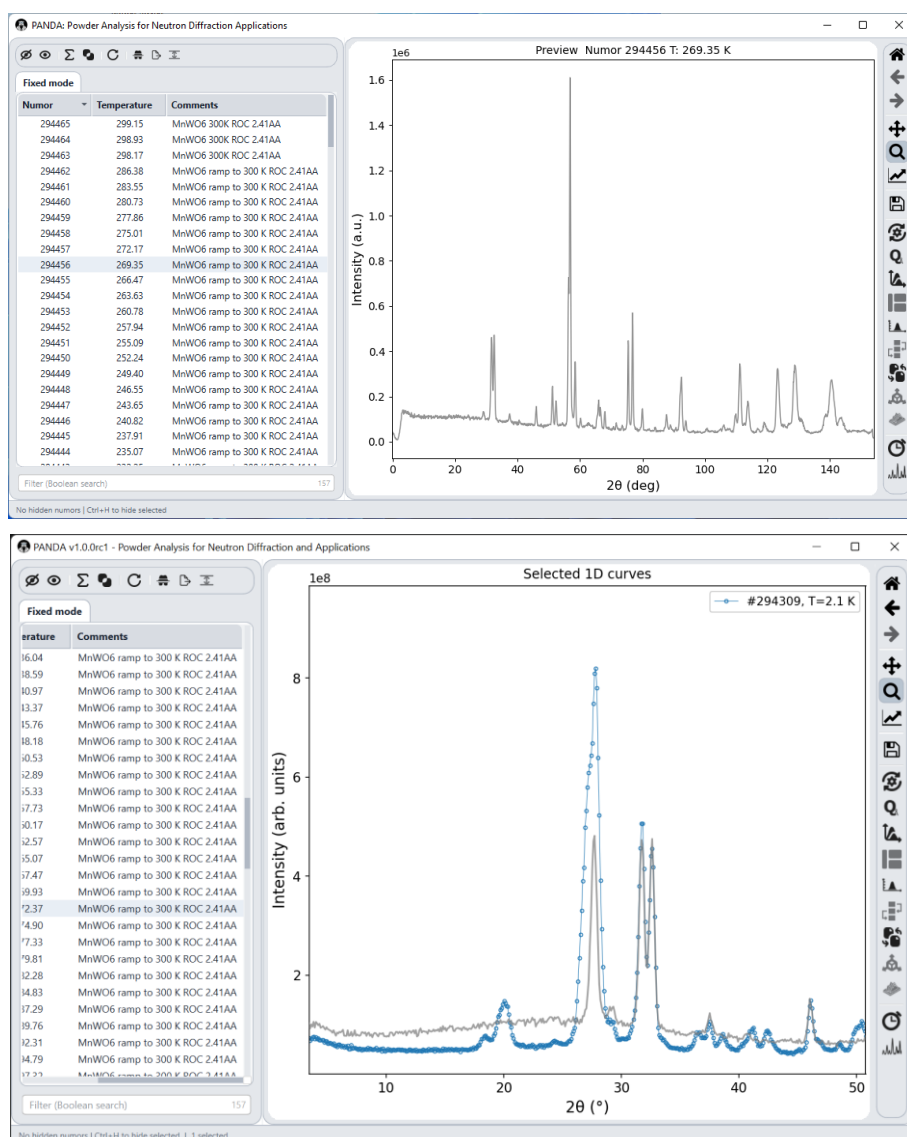
3D visualization mode showing the selected datasets, displayed as a surface+waterfall plot (right) and a OpenGL surface plot (left). Both views represent intensity as a function of 2θ and temperature, with the color scale encoding intensity from 3000 to 6000 a.u. The bottom control panel provides sliders to adjust the decimation factor (reducing the number of plotted points for performance) and the X, Y, Z scaling of the 3D view. The orientation of the 3D plot can be freely adjusted by clicking and dragging the mouse over the canvas. To exit 3D mode and return to the standard 1D or 2D view, click on any numor in the left panel.

4.5 Hover Preview

Hovering the mouse over a dataset row in the left panel shows a quick preview of that numor's diffraction pattern without changing the current selection. If a zoom is applied to a region of

interest during the preview, that zoom level is preserved as the cursor moves over other numors, allowing detailed inspection of a specific angular range across the entire dataset series. The preview remains active until the user either clicks on a numor (which switches the canvas to standard 1D mode for that selection) or right-clicks to reset the view; simply moving the mouse away from the list without clicking does not clear the preview.

When a single diffraction pattern is selected, PANDA automatically activates a comparison mode that combines the selected pattern with the hover preview functionality. In this mode, the selected pattern remains permanently displayed as a reference while hovering over other numors overlays their diffraction patterns for direct visual comparison. This feature is particularly useful for tracking subtle changes in peak position, intensity, or shape across a dataset series while maintaining a fixed reference. To avoid ambiguity, the comparison mode is automatically disabled whenever more than one pattern is selected.



Top: PANDA in hover preview mode. Moving the mouse over the numor list automatically updates the diffraction pattern displayed in the central canvas without requiring any explicit selection. The pattern is shown in grey to distinguish it from an actively selected dataset. Here, numor 294456 is being previewed. To exit hover mode and switch to standard 1D selection mode, simply click on any numor in the list. **Bottom:** Combined reference-and-hover mode. When a single diffraction pattern is selected, it remains displayed as a fixed reference while hovering over other numors overlays their diffraction patterns for direct comparison. This allows rapid inspection of changes across the dataset series while maintaining a constant reference pattern. The mode is automatically disabled when more than one pattern is selected.

5. Toolbar Actions

The top toolbar provides the main dataset operations. All actions work on the current selection in the active dataset list.



Action toolbar located at the top of the left panel, providing quick access to the main dataset operations. From left to right: Hide selected, Show all, Combine, Difference, Reload folder, Spy mode, Save log, and Edit axis.

Icon	Action	Description
	Hide selected (Ctrl+H)	Hides the selected datasets from the list and the plot without deleting them.
	Show all (Ctrl+S)	Makes all hidden datasets visible again.
	Combine (Ctrl+A)	Sums or averages two or more selected datasets. Creates a new virtual dataset in the list.
	Difference (Ctrl+D)	Subtracts datasets. Two selected: first minus second. More than two: a chosen baseline is subtracted from all the others (see 7.3).
	Reload (Ctrl+R)	Scans the project folder for new files and adds them to the list incrementally.
	Spy mode	Maximizes the dataset list and shows all available metadata columns for a detailed overview.
	Save log	Exports the current dataset list (with all visible columns) as a .log text file.
	Re-integrate 2D	Re-integrates raw 2D detector data (D2B instrument). Available only when 2D detector data is loaded.
	Motor positions	Displays a table with the main motor positions for the selected Nexus file(s). If a motor moved during the measurement, the corresponding cell shows both its initial and final positions. To view detailed information about the motor movement, right-click the table and select <i>Show Scanned Variables</i> . A new table containing the complete scan details will then be displayed.

6. Combining Datasets

The Combine function (Ctrl+A) merges two or more datasets into a single virtual dataset by summing or averaging their intensities. This is used to improve statistics by co-adding equivalent measurements.

6.1 How to Combine

1. Select two or more datasets in the list (Ctrl+Click for multi-selection)
2. Press Ctrl+A or click the Combine button in the toolbar
3. A new dataset appears in the list labeled with the constituent numors
4. The combined dataset can be plotted, exported, or used in further operations

6.2 Combination Modes

Mode	Description
Sum	Total counts are added. Suitable for increasing statistics of a single phase.
Average	Intensities are averaged. Reduces systematic offsets between equivalent scans.

6.3 Constraints

- Cannot combine datasets from different scan types (e.g., Fixed scan + 2θ scan)
- Cannot combine an already-combined dataset with a raw dataset
- All datasets must come from the same instrument

TIP: Only combine measurements collected under equivalent experimental conditions to ensure statistically meaningful results.

NOTE: When a combined dataset is created, the individual numors that contribute to it are automatically hidden from the list to keep the workspace clean and avoid confusion between raw and combined data. The original numors are not deleted and can be made visible again at any time using the Show All action (Ctrl+S) or the corresponding button in the action toolbar.

7. Difference Operation

The Difference function (Ctrl+D) subtracts one dataset from another. This is particularly useful for isolating a magnetic or structural contribution by subtracting a reference measurement (e.g., a high-temperature pattern above a phase transition).

7.1 How to Compute a Difference

1. Select exactly TWO datasets
2. Press Ctrl+D or click the Difference button
3. Result = first selected dataset minus second selected dataset
4. Error propagation is applied automatically

NOTE: The order of selection matters. The second dataset is subtracted from the first. Select carefully to get the sign of the difference you expect.

NOTE: As with the combine operation, once the difference pattern is generated the two source numors are automatically hidden to reduce clutter in the dataset list. They remain available and can be restored at any time via the Show All action (Ctrl+S) or the equivalent button in the action toolbar.

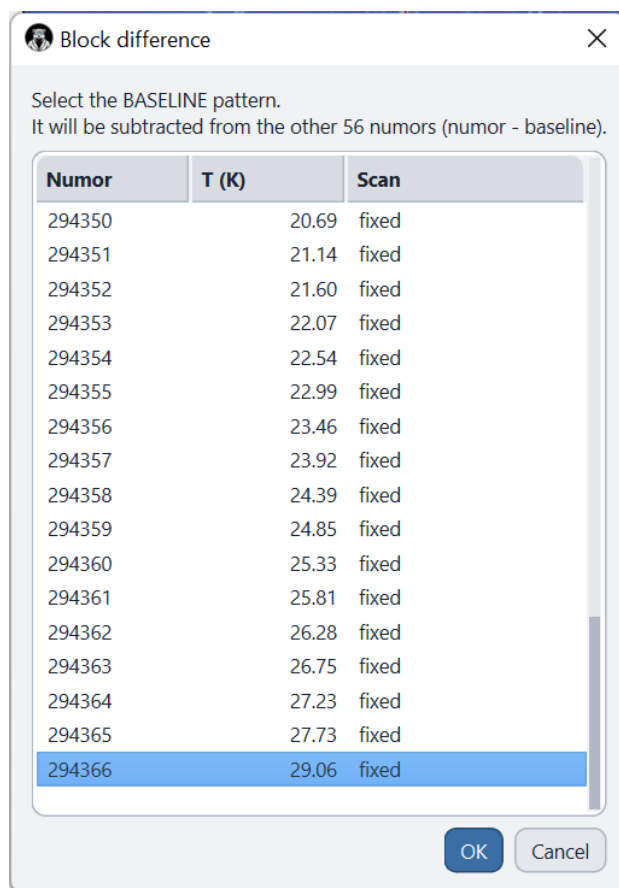
7.2 Constraints

- Exactly two datasets must be selected
- The X axes (2 θ grid) must be compatible within a small tolerance
- Cannot difference an already-differenced dataset

7.3 Block difference (ramp – baseline)

The block difference subtracts ONE reference pattern from every other selected dataset, producing one difference per numor. This is the natural tool for thermodiffraction studies, e.g., subtracting the paramagnetic pattern from a 20-numor temperature ramp to isolate the magnetic signal at every temperature.

1. Select MORE than two datasets (for example, all the numors of a ramp plus the reference pattern)
2. Press Ctrl+D or click the Difference button
3. A dialog lists the selected numors with their temperature and scan type. Choose the BASELINE, the pattern that will be subtracted from all the others, and press OK (or double-click the row)
4. PANDA creates one difference per remaining numor, named numor-baseline (e.g., 294340-294300), and places them all in a new workspace, which opens automatically



Block difference dialog (Ctrl+D with more than two datasets selected). The highlighted numor (294366, T = 29.06 K) is chosen as the baseline and will be subtracted from the other 56 numors of the ramp; the resulting differences are placed in a new workspace.

Each result keeps the temperature of its ramp numor, so the new workspace can be plotted directly as a 2D heatmap or 3D surface of the subtracted signal versus temperature. The comment column records the operation (diff: 294340-294300), and the same mathematics as the pairwise difference is applied: grid resampling when needed, full error propagation, and the automatic positive shift.

Exporting the numors of the new workspace follow the same rules than whatever other numor.

NOTE: The baseline is only subtracted from datasets of its own scan type (fixed, 2θ scan or special scan). Numors of a different scan type, as well as already-differenced datasets or patterns with no angular overlap, are skipped and reported in the console, never aborting the whole operation.

NOTE: Unlike the pairwise difference, the source numors are NOT hidden after a block difference: the original ramp remains intact in its tab, and the results live in their own workspace.

8. Automatic Background Subtraction

Estimates and subtracts an instrumental or diffuse background from every selected numor, producing one corrected dataset per pattern (`{numor}_nbkg`) gathered in a new workspace.

The background is estimated from the pattern itself, so no reference measurement is required. Seven estimation methods are available, from asymmetric least-squares smoothing to Chebyshev polynomials with user-defined anchor points, covering both the smooth instrumental backgrounds of a well-shielded setup and the strong, structured diffuse scattering produced by hydrogen-containing samples.

A single dialog drives the whole operation: the method and its parameters are chosen once and applied to the entire selected block, while a live preview shows the estimated background superimposed on any one of the selected patterns. This makes the correction reproducible across a ramp, every numor is treated with identical settings, while still allowing the result to be inspected pattern by pattern before it is committed.

The source numors are neither hidden nor modified: the original datasets remain visible in their tree, and the corrected copies are collected in a new workspace that opens automatically. Each corrected dataset keeps the metadata of its parent numor, uncertainties and temperature, so the new workspace can be plotted as a 2D heatmap, exported, or used in a subsequent difference operation exactly like any other workspace.

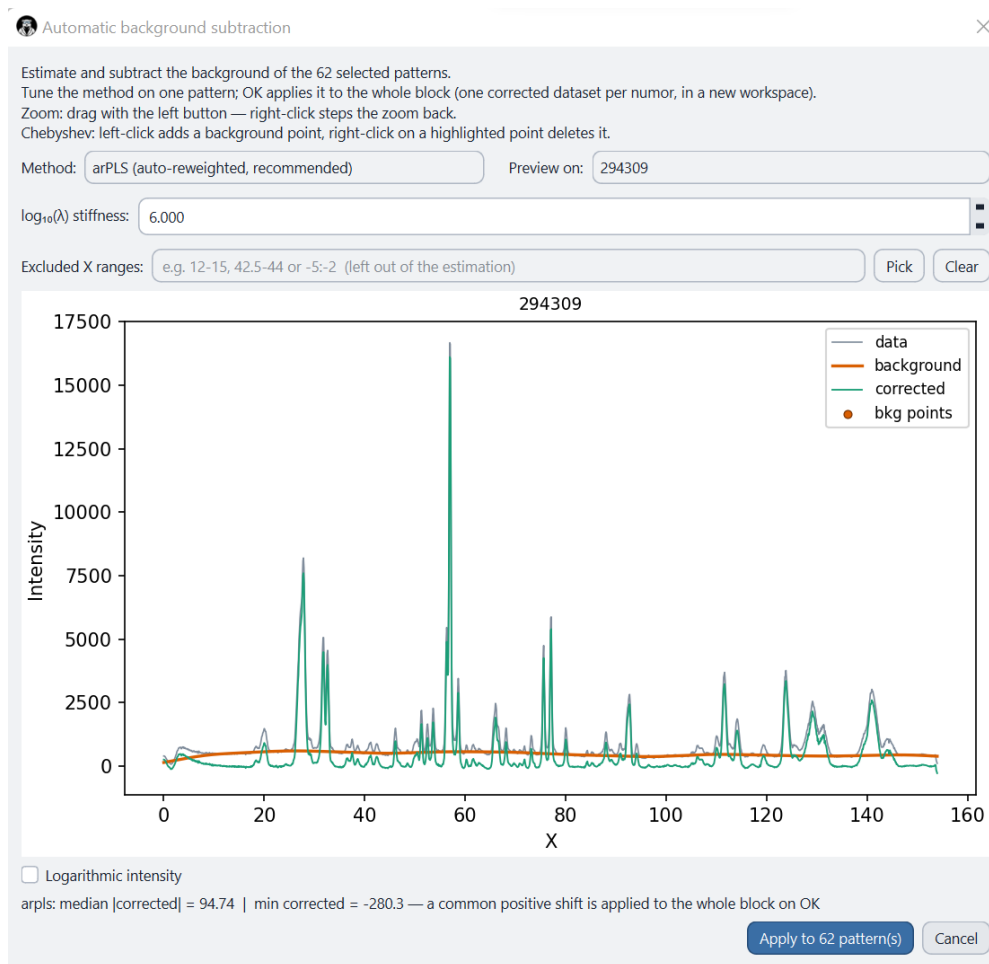
When to use this approach

Estimating the background from the data themselves is an approximation. It is the appropriate tool when the background is a nuisance to be removed so that the signal can be seen, compared or measured:

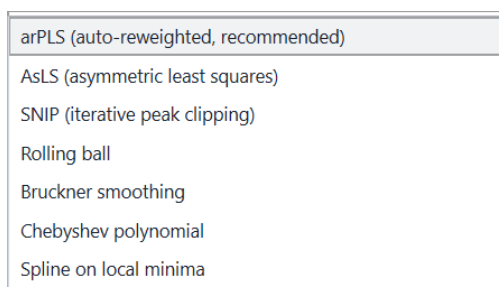
- Visual inspection and presentation. Comparing patterns of a ramp on a common scale, producing heatmaps in which weak reflections are not drowned by a slowly varying background, or preparing figures.
- Following peaks across a series. Tracking the appearance, position or intensity of a reflection as a function of temperature, pressure or time, where the quantity of interest is the relative change rather than an absolute structure factor.
- Integrated intensities of individual peaks, when the background under the peak is smooth on the scale of the peak width and no empty-container measurement is available.
- Samples with strong incoherent scattering, typically hydrogen-containing, where the background is intense and structured and a low-order polynomial fitted during refinement struggles to describe it.

8.1 How to Subtract a Background

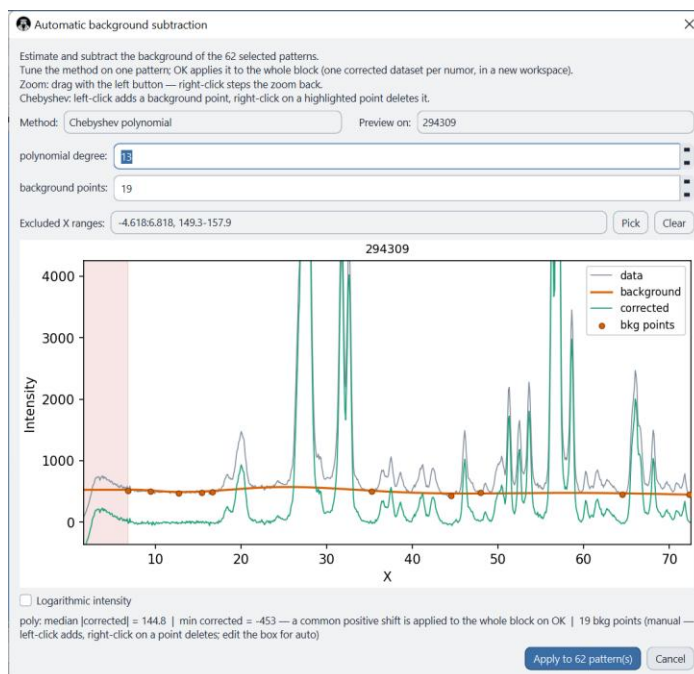
- Select the numors to correct in any tree. Use individual patterns, or Ctrl+Click to select a contiguous block such as a complete temperature ramp. All selected patterns are corrected with the same method and the same parameters, so the block should be homogeneous, one ramp, one sample, one instrument configuration.
- Click the background button in the right-hand toolbar.  The dialog opens with a live preview already displayed on one of the selected patterns, showing the measured pattern, the estimated background superimposed on it, and the corrected result.



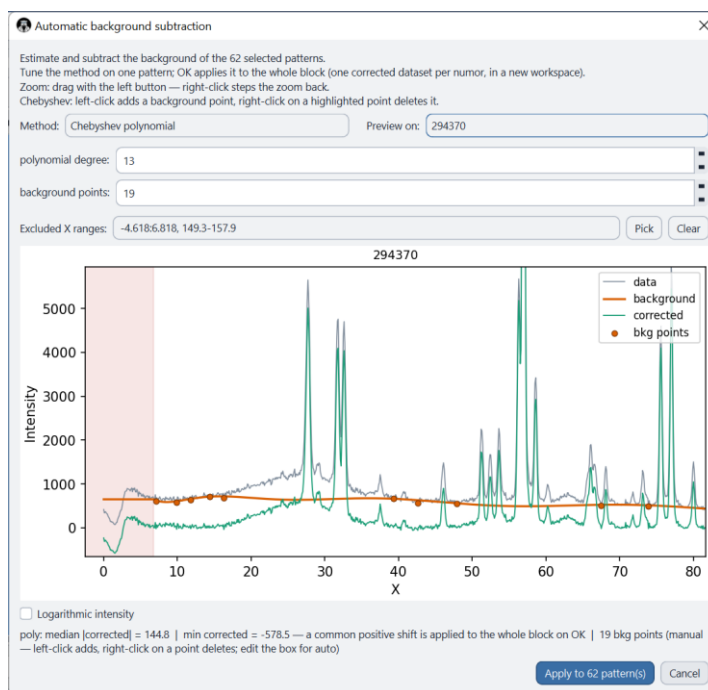
- Choose the estimation method from the method selector. The parameter fields update to those of the selected method, and the preview is recomputed as soon as any of them changes.



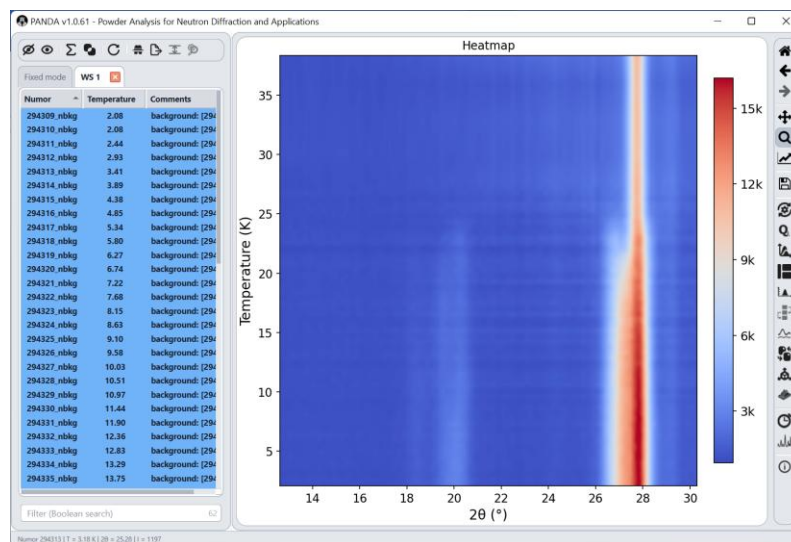
- Tune the parameters while watching the preview. The aim is a background that follows the baseline between reflections without climbing into the peaks. Zooming into a region of interest and excluding ranges where the background changes abruptly usually helps more than pushing a single parameter to an extreme value.



- Check the preview on several patterns of the block. Change the previewed pattern to a few representative points of the ramp, the first, the last, and one where the diffraction pattern changes most. Parameters that work on one pattern do not necessarily work on all of them, and this is the only opportunity to notice it before the correction is applied.



- Apply the correction with the button that reports how many patterns will be processed. PANDA estimates and subtracts the background for every selected numor, applies the common positive shift, and collects the results in a new workspace named after the source selection. The workspace opens automatically once processing finishes.



The corrected datasets are named {numor}_nbkg and keep the uncertainties and the temperature of their parent numor. The original numors remain visible and unmodified in their own tree, so the correction can be repeated with different settings without reloading anything: simply reselect the original block and open the dialog again. Each run produces its own workspace, which makes it practical to compare two methods side by side before deciding which one to keep.

8.2 Estimation Methods

Seven methods are available. They differ in how they decide what is background and what is signal, and therefore in how they fail. The parameter names below follow the dialog; the typical values are starting points, not prescriptions.

Method	How it works	Main parameters	Best suited to	Fails by
arPLS	Fits a smooth curve through the data by penalised least squares, weighting points below the curve much more heavily than points above it. The weights are recomputed automatically at each iteration from the noise level, so peaks progressively stop pulling the curve upwards.	Smoothness (λ)	Almost any pattern. Curved, structured backgrounds including strong incoherent scattering. Good default because it needs no asymmetry parameter.	Absorbing broad peaks if the smoothness is set too low.
AsLS	The same penalised-smoothing idea, but	Smoothness (λ),	Cases where arPLS is either too rigid or too permissive and the	Being sensitive to the asymmetry value: too high lifts

Method	How it works	Main parameters	Best suited to	Fails by
	the asymmetry between points above and below the curve is fixed by the user instead of being derived from the noise.	asymmetry (p)	balance needs to be forced by hand.	the background into the peaks, too low flattens it against the lowest points.
SNIP	Iteratively clips peaks: each point is compared with the mean of two neighbours at a given distance and replaced by the smaller of the two. Repeating this with decreasing distances erodes anything narrower than the window, leaving the background.	Window width	Patterns with many narrow, well-defined reflections. Fast and robust.	Removing any feature narrower than the window, broad peaks and amorphous haloes disappear.
Rolling ball	Rolls a ball of fixed radius along the underside of the pattern; the envelope traced by its top is the background. Formally a morphological opening followed by smoothing.	Ball width, smoothing width	Quick, intuitive corrections when the background is smooth and the peaks are narrow.	Being very sensitive to the width: too small it follows the peaks, too large it cuts corners under curved backgrounds.
Bruckner smoothing	Repeatedly smooths the pattern and keeps, at each point, the smaller of the smoothed and the current value, so peaks are progressively shaved off from the top down.	Window width, iterations	Classical powder patterns; behaves similarly to SNIP and is a useful cross-check against it.	Converging slowly, and by eroding broad features when many iterations are used.
Chebyshev polynomial	Fits a polynomial to the whole pattern, discarding points that lie above the fit and refitting until only the baseline contributes. Anchor points can be added manually to force the polynomial through positions known to be background.	Degree, background points	Smooth instrumental backgrounds, and any case where the background must be controlled explicitly. The only method offering manual anchor points.	Oscillating between anchors at high degree, and by riding up on the overlapping tails of dense patterns — it has no local notion of baseline.
Spline on local minima	Selects the lowest point within each of a series of intervals and interpolates a smooth cubic curve through them.	Number of anchors / interval width	Reproducible, easily understood corrections; useful when the result must be explained or defended point by point.	Following the noise downwards, since the minimum of an interval is a biased estimate of the baseline; and by sagging where an interval contains no true background.

8.3 Live Preview: Zoom and Region Exclusion

The preview shows the selected pattern, the estimated background superimposed on it, and the corrected result. It is recomputed every time a parameter changes, so the effect of each adjustment is visible immediately.

Zoom

Left-drag on the plot to zoom into a region.

Right-click steps back one zoom level; repeated clicks return to the full view once the history is empty.

Changing the previewed pattern resets the zoom to the full range.

Zooming affects only the display. The background is always estimated over the whole pattern, never over the visible range alone.

Excluded regions

Regions where the background changes abruptly, or where a strong feature would drag the estimate upwards, can be excluded from the estimation. Two ways to define them:

Type the ranges in the exclusion field, separated by commas: 12-15, 42.5-44.

Click Pick: the button turns red and reads Picking..., then drag on the plot to define a range. Repeat for further ranges, and click Pick again to leave the mode.

Excluded ranges are shaded red on the plot. Points inside them are ignored when the background is fitted, and the background is interpolated across the gap. The subtraction itself still covers the whole pattern: excluding a region removes it from the fit, not from the correction.

8.4 Manual Background Points (Chebyshev)

When the Chebyshev method is selected, the preview shows a set of orange dots: the points the polynomial is forced to pass through. PANDA detects them automatically, but they can be edited by hand whenever the automatic estimate misses the baseline in a particular region.

Editing points

Hovering over a point highlights it with a red ring.

Left-click without dragging adds a point at the cursor position. (Dragging is interpreted as a zoom, so the click must be stationary.)

Right-click on a highlighted point deletes it. Deletion is refused when it would leave fewer points than the polynomial degree plus one, since the fit would then be undetermined.

The background points field mirrors the current count. Editing it directly discards the manual points and returns to automatic detection.

Safety net across the block

The points are placed on the previewed pattern, but they are applied to every pattern of the selection, and a position that sits on the baseline in one pattern may fall on a reflection in another. To prevent this, on every other selected pattern each point is allowed to slide to the nearby data sample whose intensity is closest to the value it had on the reference pattern.

The reference is always the pattern on which the points were defined, never the previously corrected one, so the displacements cannot accumulate along a ramp.

This handles the common case of a reflection that appears or shifts onto a fixed point, a magnetic peak growing below a transition, for example, which would otherwise drag the background upwards on part of the series only.

NOTE: *The safety net is a local correction, not a guarantee. Before applying, change the previewed pattern to a few points of the ramp and confirm that the orange dots still sit on the baseline in each of them, particularly where the diffraction pattern changes most.*

8.5 Positive Shift and Constraints

A single positive shift is applied to the whole block. Once all patterns have been corrected, PANDA finds the most negative corrected value across the entire selection and adds that amount, as a constant, to every point of every pattern. The result is that no corrected intensity is negative while the relative intensities are preserved, within a pattern, because the same constant is added to all its points, and between patterns, because the same constant is used for all of them. A shift computed separately for each pattern would not have this property.

Two consequences follow:

The corrected data are offset from zero by a known constant. Any analysis that assumes a zero baseline must account for it; in a refinement, the shift should be declared together with the subtracted background as a fixed background contribution.

The uncertainties are unchanged. Adding a constant does not alter the variance, so the sigma of each point is carried over from the parent numor.

9. Peak Fitting

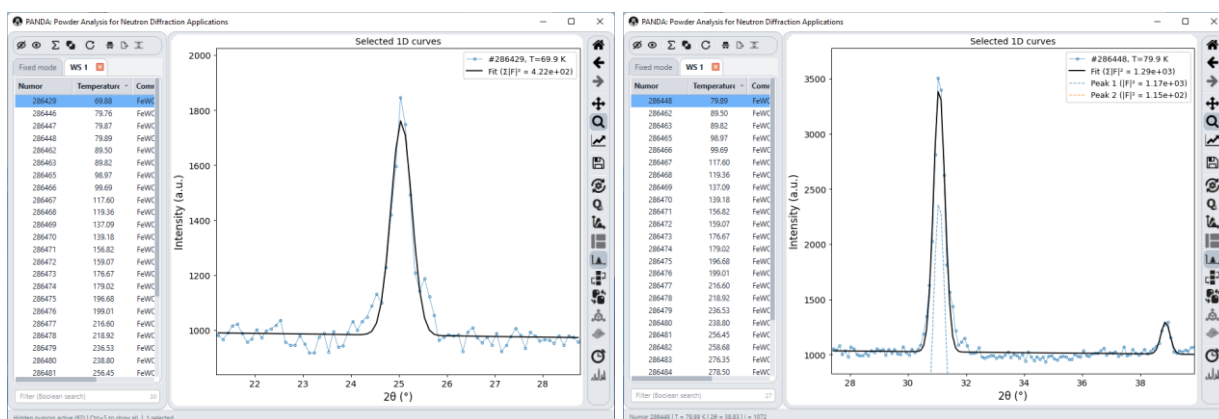
PANDA includes an interactive peak fitting module for 1D diffraction patterns. It supports Gaussian peak models with a linear or constant background.

9.1 Activating Fit Mode

1. Select a single dataset
2. Click the Fit button in the right toolbar
3. The canvas enters Fit mode; the zoom range is locked to the current view

9.2 Defining Peaks

- Click on the left and right of the peak to select a starting background
- Click on a peak position in the plot to add a Gaussian peak
- Each click adds a new peak centered at the clicked position
- The fit is updated interactively after each addition



Peak fitting mode activated on numor 286429 ($T = 69.9$ K), shown in workspace WS 1. The zoomed view is locked to the $21-29^\circ$ 2θ region of interest. The fitted Gaussian peak (black line) has been defined by first clicking on either side of the peak to set the background level, then clicking on the peak position to place a Gaussian component centered at $\sim 25^\circ$ 2θ . The fit is updated interactively after each click. The legend reports the integrated structure factor ($\sum |F|^2 \approx 4.22 \times 10^2$), providing an immediate quantitative estimate of the peak intensity. The dataset list in the left panel (WS 1 tab) shows the 30 numors available for sequential fitting.

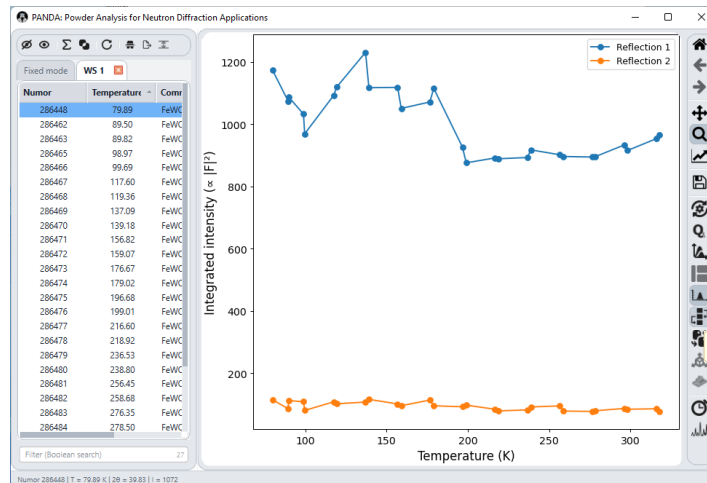
9.3 Fit Results

The following parameters are extracted for each fitted peak:

- Peak center (2θ or Q)
- Peak width (FWHM)
- Integrated intensity

9.4 Sequential Fit

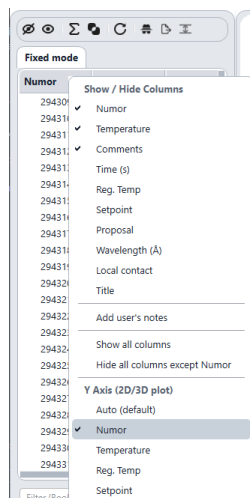
Once a peak model is defined on one dataset, the Sequential Fit button propagates the fit across all visible datasets in the current list, applying the same peak model and extracting fit parameters as a function of temperature.



Sequential fit results displayed in PANDA (workspace WS 1), showing the temperature evolution of the integrated intensity ($\Sigma |F|^2$) for two fitted reflections across 27 numors spanning ~70–320 K. Reflection 1 (blue) exhibits a clear intensity decrease with increasing temperature, while Reflection 2 (orange) remains comparatively weak and approximately constant throughout the temperature range. Results are automatically saved to the working folder for further analysis.

TIP: The sequential fit results are automatically saved to the working folder defined when loading the data, and can be further used for analysis of lattice parameter or peak intensity evolution.

The X-axis used in sequential *Fit mode* depends on the parameter currently selected as the vertical axis in the 2D or 3D visualizations. Whenever a different parameter (e.g. Numor, Temperature, Time, Reg. Temp and Setpoint) is selected for the heatmap Y-axis, the same parameter is automatically used as the X-axis for all subsequent sequential fits. This ensures that the fit results remain consistent with the current selected data representation.



Changing the parameter used as the X-axis. Right-click the table header to open the context menu and select the desired parameter. The selected parameter is automatically applied to the 2D and 3D visualizations and, consequently, becomes the X-axis used in *Fit mode*.

Fit Result Indicators

PANDA displays different markers in the fit plot to indicate the quality and reliability of each fitted point.

- **Successful fit** – When the fit converges and the estimated parameter uncertainty is below 50%, the result is displayed as a coloured circle with error bars. These points are considered reliable.
- **Low-confidence fit** – If the fit converges but the estimated uncertainty exceeds 50% of the fitted value, the result is displayed as a coloured cross (×) without error bars. These points should be interpreted with caution.
- **Fit not converged** – Once the fitting procedure fails to converge for a dataset, the last available fitted values are retained and displayed as grey points without error bars. This allows the user to identify where the automatic fitting procedure stopped producing reliable results.
- **Fit failed** – If the fitting algorithm cannot determine a solution (for example, due to a numerical failure), no point is displayed for that dataset.

10. Exporting Data

10.1 Export Figure

The Export button in the right toolbar saves the current plot as an image file (PNG, PDF, or SVG). A file dialog allows choosing the output path and format.

TIP: Use vector formats (PDF or SVG) for publication-quality figures. PNG is suitable for quick sharing and presentations.

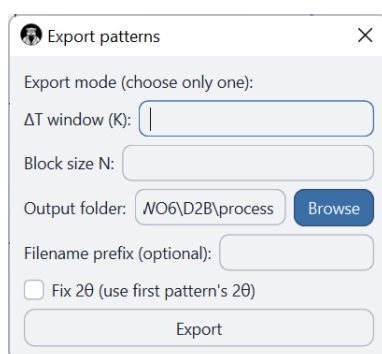
10.2 Save Log

The Save Log action (toolbar) exports the content of the current dataset list to a plain text .log file. The log includes numor, temperature, comments, and any additional columns currently visible in the list. For a complete experiment record, the Save Log action can be combined with Spy mode: activating Spy mode first exposes all available metadata columns, so that the exported log captures the full set of experimental parameters in just a few clicks.

10.3 Export Pattern

The Export Patterns dialog allows exporting the selected diffraction patterns to individual files in a format compatible with Rietveld refinement software such as FullProf, JANA or GSAS. It is

accessible from the toolbar  and opens the dialog shown below.



Export patterns dialog in PANDA. The window provides different export modes for temperature-series diffraction data, including export over a selected ΔT temperature window or grouping datasets into blocks of fixed size N. Users can define the output directory and optional filename prefix, and optionally force all exported datasets to use the 2θ grid of the first pattern to ensure angular consistency across the exported series.

Two mutually exclusive binning strategies are available:

- **ΔT window (K):** Groups patterns by temperature intervals of the specified width. All patterns whose temperature falls within the same window are averaged and exported as a single file. This mode is suited for experiments where temperature is the scanned variable and a coarser thermal grid is desired for the refinement.

- **Block size N:** Groups patterns into consecutive blocks of N patterns regardless of temperature, and exports one averaged file per block. Use this mode when a fixed number of patterns per output file is more appropriate than a temperature-based criterion.

Only one of the two fields should be filled. If both are left empty, patterns are exported individually with no binning, preserving a one-to-one correspondence between input patterns and output files. Filling both fields simultaneously will result in an error.

Output folder: The destination directory for the exported files. The current path is shown in the text field and can be changed via the Browse button, which opens a standard folder selection dialog.

Filename prefix (optional): A custom string that will be prepended to each output filename. If left empty, a default naming scheme based on the numor or dataset identifier is used. Providing a prefix is recommended when exporting multiple datasets to the same folder to avoid name collisions.

Fix 2θ (use first pattern's 2θ): When this checkbox is active, the 2θ axis of the first pattern in the selection is used as the common angular grid for all exported files. Subsequent patterns are interpolated onto this grid before averaging. This ensures that all output files share an identical angular axis, which may be required by some refinement or visualization programs when working with heatmap files. If the checkbox is left inactive, each exported file retains its own native 2θ grid.

Export: Clicking “Export” writes the output files to the selected folder.

TIP: For sequential refinements in FullProf, enable *Fix 2θ (optional)* and use a filename prefix with the sample name and experimental condition (e.g. `MySample_ramp_10K_to_300K`) to keep the output folder organised. PANDA will automatically add a numeric counter suffix required for sequential refinement (e.g. `MySample_ramp_10K_to_300K_001 ... MySample_ramp_10K_to_300K_999`).

10.3.1 Output file naming

The name of each exported file is built according to three rules, in order of precedence:

1. *Filename prefix given:* every file is named `prefix_NNN.xys`, where NNN is a sequential counter following the selection order (e.g. `FeWO4_ramp_001.xys`, `FeWO4_ramp_002.xys`).
2. *Dataset renamed by the user:* datasets created inside PANDA (combine, difference, block difference) can be renamed by double-clicking their name in the dataset list. A renamed dataset exports under exactly that name plus the temperature tag, with no counter: renaming a difference to `CsRb_20_1p28_2K` produces `CsRb_20_1p28_2K_T2.00.xys`. Block-difference results follow this rule automatically with their numor-baseline names (e.g. `294340-294300_T16.07.xys`). A counter is re-added only if two exported files would otherwise collide (same name and same temperature).
3. *Default:* raw numors export as `numor_Ttemp_NNN.xys` (e.g. `294340_T16.07_001.xys`); the temperature tag is omitted when no temperature is available.

Alongside the patterns, PANDA writes a `buffer.buf` file listing every exported filename in order, ready to be used as the input list for sequential FullProf refinements

10.4 Integration with pyPRF

The pyPRF button  in the PANDA toolbar opens pyPRF, an interactive viewer for the .prf output files generated by FullProf after a refinement. pyPRF is designed for rapid visualisation and publication-quality export of refinement results, and runs as an independent window alongside PANDA.

10.4.1 Requirements and installation

pyPRF is a self-contained Python script. To run it independently (without PANDA), install the required packages with pip:

```
pip install numpy matplotlib PySide6
```

To enable Word export of refinement reports, also install:

```
pip install python-docx
```

Library	Minimum recommended version
Python	3.10+
numpy	1.24+
matplotlib	3.7+
PySide6	6.4+
python-docx	any recent version (optional)

Once the dependencies are satisfied, launch pyPRF with:

```
python main.py
```

On startup, pyPRF prints the detected versions of Python, numpy, matplotlib and PySide6 to the console to assist in diagnosing any incompatibility.

TIP: When pyPRF is launched from PANDA, it reuses the existing QApplication instance and automatically adopts the active theme (light/dark) of the parent window.

10.4.2 Interface layout

The pyPRF window is divided into three main panels separated by resizable splitters. Each panel width can be adjusted by dragging the handle between panels.

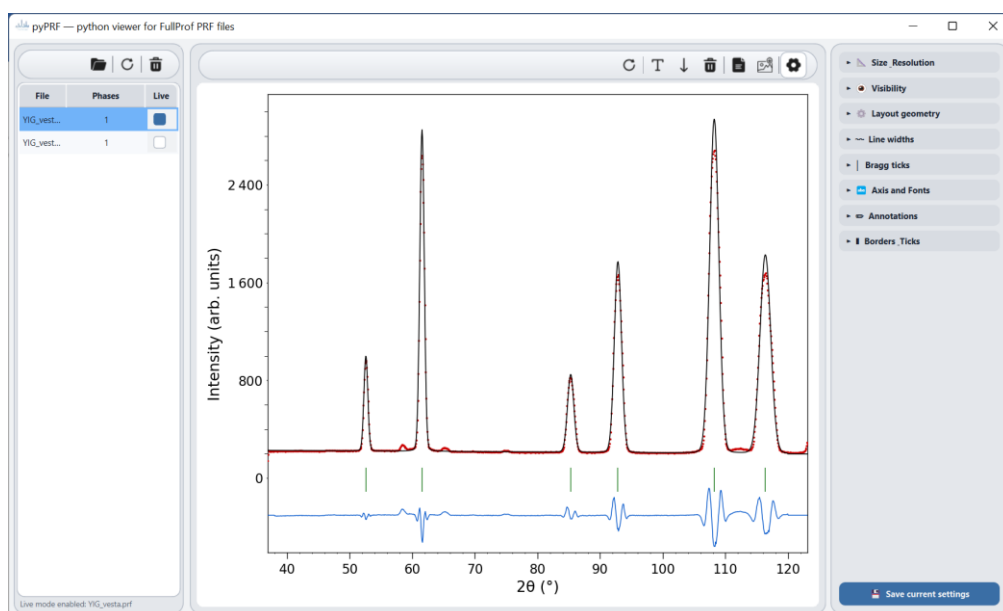
Panel	Location	Primary function
File list	Left	Load, remove and select .prf files; Live mode toggle
Plot canvas	Centre	Refinement visualisation; zoom, pan, annotations
Plot settings	Right	Collapsible sections controlling all visual appearance

Left panel — file list

Displays the loaded .prf files in a table with three columns: filename, number of phases, and a per-file Live toggle button.

- To load a file, click Add file (.prf) at the top of the panel and select one or more .prf files from the open dialog.
- Click any row to select that file and plot it on the central canvas. The selected row is highlighted in blue.
- To remove a file from the list, select it and click Remove file.
- On startup, pyPRF automatically restores all .prf files from the last used directory, so files do not need to be reloaded manually at each session.

TIP: Live mode: When Live mode is active (blue indicator), pyPRF monitors the file on disk using QFileSystemWatcher and reloads it automatically every time FullProf updates it, enabling real-time monitoring of an ongoing refinement without manual intervention.



General view of the pyPRF interface showing its three main panels: the left panel listing the loaded PRF files with their number of phases and the per-file Live toggle (shown active in blue for the selected file); the central panel displaying the result of the last refinement plot with the observed data (red dots), calculated profile (black dashed line), and Bragg reflection tick marks (green), together with the difference curve (blue line) offset below the main profile; and the right panel containing the collapsible sections for fine-grained control of the plot appearance.

Central panel — plot canvas

Shows the refinement fit. The toolbar above the canvas provides navigation and editing actions.

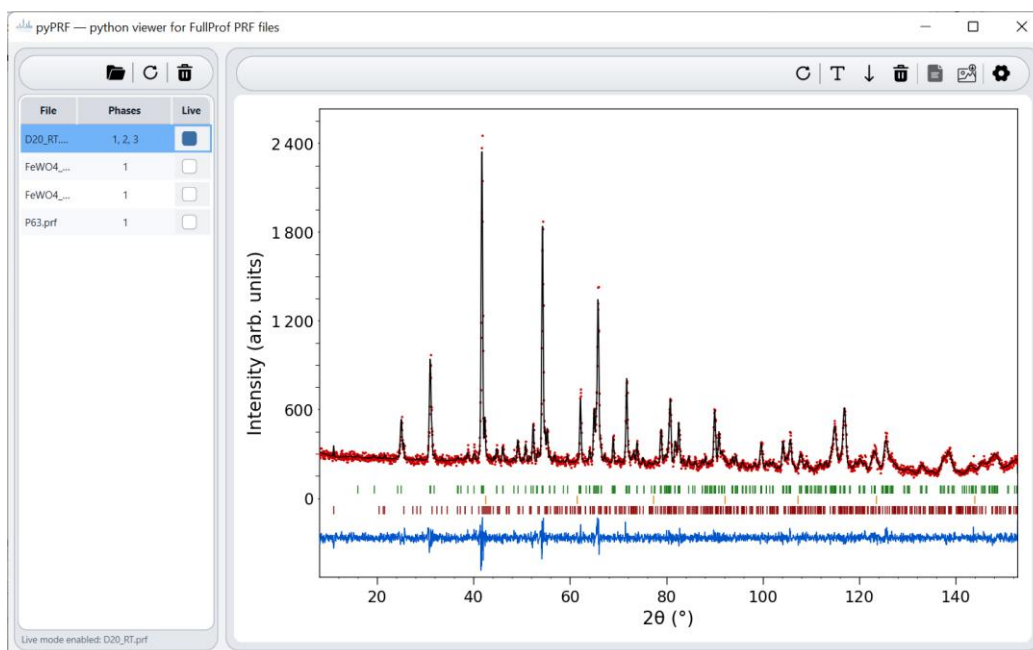
- **Powder:** observed data (dark red), calculated profile (black dashed line), difference curve (blue) and Bragg tick marks (green and other colours) indicating the allowed reflections for each phase.
- **Single-crystal:** Four alternative views are available — F^2_{obs} vs F^2_{cal} , F_{obs} vs F_{cal} , $F_{\text{obs}} - F_{\text{cal}}$ vs. $\sin(\theta)/\lambda$; and, $F^2_{\text{obs}} - F^2_{\text{cal}}$ vs. $\sin(\theta)/\lambda$ scatter plot.
- **Zoom:** scroll the mouse wheel to zoom in or out; right-click to reset the view to full extent.
- **hkl tooltip:** hovering over a Bragg tick mark displays a popup with the hkl indices of the corresponding reflection.

Right panel — plot settings

Contains collapsible sections that control all visual aspects of the figure. Each section can be expanded or collapsed by clicking its header button. Any change is applied immediately without requiring confirmation.

Section	Available controls
Size & Resolution	Figure width and height (inches), export DPI
Visibility	Legend, title, background line, excluded regions, clipping of excluded data
Layout geometry	Residual shift, Bragg tick band position and height
Line widths	Base width; observed line/points, calculated, difference, background
Bragg ticks	Tick line width and relative height
Axis and Fonts	Font family, axis label and tick sizes; axis label text (LaTeX supported)
Annotations	Text font, size, style and colour; arrow colour, width and head size
Borders & Ticks	Individual spine visibility, spine width and colour; major/minor tick size and colour
Single crystal	Visible only for single-crystal datasets, this panel offers four alternative diagnostic plots for comparing observed and calculated structure factors

At the bottom of the right panel, the Save current settings button persists all parameters to the system registry (QSettings) for use in future sessions.



pyPRF viewer showing the refinement results for powder and single crystal datasets. The main panel displays the standard powder diffraction fit plot: observed data (red dots), calculated profile (black line), and difference curve (blue line) at the bottom. The tick marks below the profile indicate the allowed Bragg reflections for each phase (green, dark red, and dark green rows). The left panel lists the loaded PRF files with their associated number of phases and a Live mode toggle, which automatically reloads the refinement output as FullProf updates it, enabling real-time monitoring of an ongoing refinement. The top toolbar provides access to export, table generation, and visualization options.

10.4.3 Canvas toolbar

The toolbar at the top of the central panel provides the following actions:

Button	Action
↺ Reset view	Restores the full zoom and pan extent for the current file
T Text	Activates text annotation mode; click on the plot to place a label (toggle)
↗ Arrow	Activates arrow annotation mode; click once for the tail, again for the head (toggle)
✕ Delete annotation	Removes the selected annotation; if none is selected, removes all annotations
■ Report	Opens the refinement report viewer from the associated .sum file
📄 Export figure	Opens the save dialog to export the figure in the chosen format
⚙ Settings	Shows or hides the right settings panel (toggle)



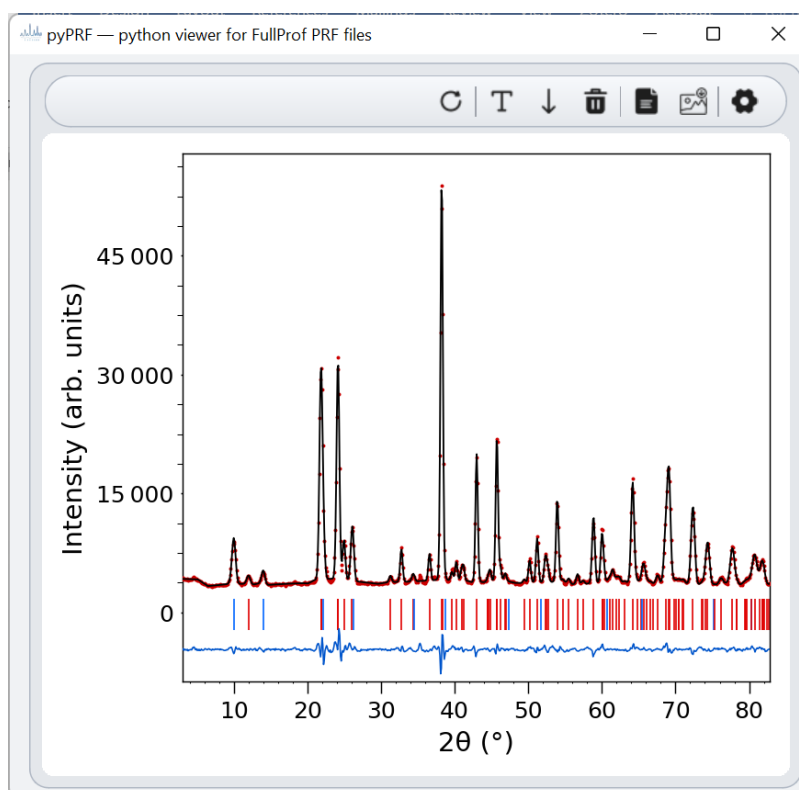
View of the toolbar available. From left to right: refresh the display, edit the plot title, export the current figure, delete the selected item, open the report window, insert an image into the report, and access the settings menu. The available actions operate on the currently active figure and associated analysis results.

TIP: Annotation modes: The Text and Arrow buttons are mutually exclusive: activating one deactivates the other. The cursor changes to a crosshair (+) when annotation mode is active. Press the same button again, or right-click on the canvas, to exit annotation mode.

10.4.4 Powder diffraction data representation

For powder diffraction datasets, pyPRF displays the standard Rietveld representation. The figure contains, from top to bottom:

- **Observed data** (dark red, #CC0000): plotted as a continuous line or as individual points, depending on the setting in the Line widths panel. Marker size and line width are independently configurable.
- **Calculated profile** (black, dashed line): includes the background contribution when available in the .prf file.
- **Difference curve** (blue): $Y_{obs} - Y_{cal}$, centred on zero (pyPRF removes the background offset by subtracting the median of the residual). Its vertical position is controlled by the Residual shift parameter.
- **Bragg tick marks** (green, dark red, cyan... for each phase): vertical segments at the positions of the allowed reflections. Hovering over a tick displays the hkl indices in a popup.
- **Excluded regions** (semi-transparent grey bands): 2θ intervals excluded from the refinement, read directly from the .prf file header.



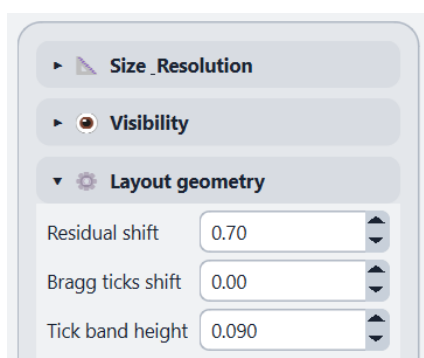
Example of a pyPRF refinement window showing the observed diffraction pattern (red symbols), calculated profile (black line), Bragg reflection positions (red and blue tick marks), and difference curve (blue line). The toolbar at the top provides quick access to display, export, reporting, and configuration functions.

TIP: Background line: Enabling the Background line option in the Visibility section overlays the calculated background in grey dashed style on the main profile, allowing visual assessment of the relative importance of the background.

Vertical layout geometry

The vertical positions of the difference curve and the Bragg tick band are controlled independently by three parameters in the Layout geometry section of the right panel:

Parameter	Description
Residual shift	Additional downward shift of the difference curve, scaled by the residual amplitude. Value 0 produces the automatic default positioning.
Bragg ticks shift	Downward shift of the Bragg tick band from the pattern base, scaled by the intensity range yrange.
Tick band height	Height of the Bragg tick band as a fraction of yrange. With multiple phases, the band is divided equally among them.



Detail of the Layout Geometry settings used to adjust the position of the residual curve, Bragg reflection ticks, and tick band height.

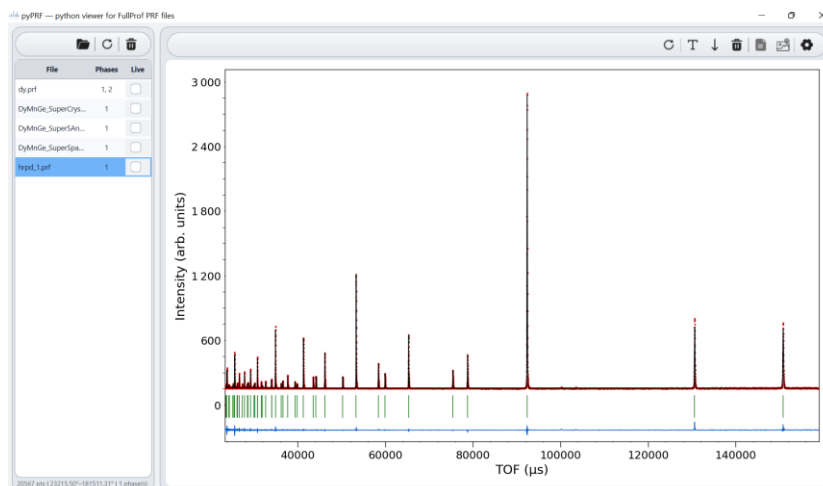
The pattern is shifted upward automatically to ensure the data region never overlaps with the Bragg tick band; no manual adjustment is required.

10.4.5 Time-of-flight (TOF) data

pyPRF natively supports TOF refinements generated with the PRF=3 option of FullProf. The representation is identical to that of conventional powder data, with the sole difference that the horizontal axis is expressed in microseconds (μs).

Axis type detection is automatic: pyPRF analyses the range of values in the first column of the .prf file and sets the horizontal axis label accordingly. All pyPRF features, Live mode, refinement report viewer, plot settings, and figure export, are fully available for TOF datasets.

TIP: If the X-axis label does not match the data type correctly, you can edit the text in the X field of the Axis and Fonts panel. LaTeX notation is supported using the $\$...\$$ syntax.



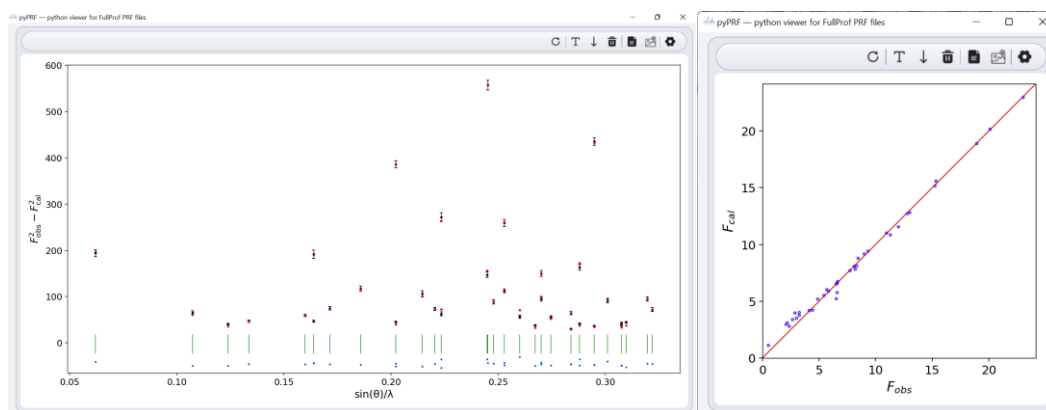
pyPRF displaying a TOF (time-of-flight) refinement result from a FullProf PRF file generated with PRF=3. The horizontal axis is expressed in microseconds (μs) and the plot follows the standard Rietveld representation: observed data (red dots), calculated profile (black dashed line), difference curve (blue line), and Bragg reflection tick marks for each phase (green and cyan rows).

All pyPRF features — Live mode, refinement report viewer, plot settings, and figure export — are fully available for TOF datasets.

10.4.6 Single-crystal data representation

For single-crystal .prf files (detected automatically by the presence of the $\sin(\theta)/\lambda$ or Gobs/Gcal column), pyPRF offers four view modes selectable from the Axis and Fonts section of the settings panel or from the toolbar options:

Mode (mono_view)	Description
$F^2_{\text{obs}} - F^2_{\text{cal}}$ vs. $\sin(\theta)/\lambda$	Standard difference view in terms of squared structure factors. Includes error bars (sigma) and Bragg tick marks.
$F_{\text{obs}} - F_{\text{cal}}$ vs. $\sin(\theta)/\lambda$	Same as stl but using F amplitudes (square root of F^2). Error propagation is applied automatically: $\sigma(F) = \sigma(F^2) / (2F)$.
F^2_{obs} vs. F^2_{cal}	Scatter plot for evaluating the correlation between observed and calculated values. The identity line is drawn and data are shown as open circles.
F_{obs} vs. F_{cal}	Same as scatter but using F amplitudes.

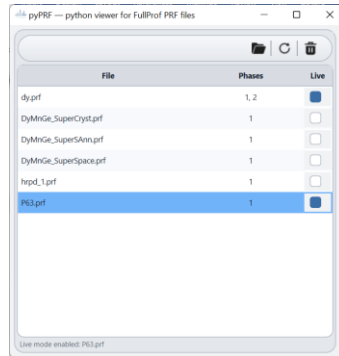


Examples of different single-crystal diffraction data representations available in pyPRF

TIP: Dubious reflections: Reflections flagged as dubious in the .prf file (column iv $\neq$ 1) are highlighted in the tooltip to facilitate their identification.

10.4.7 Live mode: real-time monitoring

Live mode allows an ongoing refinement to be monitored without reloading the file manually. When active, pyPRF uses QFileSystemWatcher to detect any modification of the .prf file on disk and updates the plot automatically.



pyPRF file manager with **Live Mode** enabled. The selected PRF file is automatically reloaded whenever it is modified, allowing real-time monitoring of the refinement progress.

Enabling and disabling

- Click the Live button in the corresponding column of the file list in the left panel.
- The indicator turns blue when Live mode is active and grey when inactive.
- Each file in the list has its own independent Live toggle, allowing multiple files to be monitored simultaneously.

Internal behaviour

The reload system is designed to be robust against the incremental updates that FullProf performs during a refinement:

- After detecting a file change, pyPRF waits a short stabilisation period (debounce of approximately 120 ms) to ensure that FullProf has finished writing the file before reading it.
- If reading fails — for example because the file is still being written — pyPRF retries automatically.
- The current annotations and zoom level are preserved between updates, so the view does not need to be readjusted after each refinement cycle.

TIP: Use Live mode during an active FullProf refinement to monitor the fit evolving in real time. Once convergence or the maximum number of refinement cycles is reached, deactivate Live mode and proceed with the export steps described below.

10.4.8 Refinement report viewer

The report viewer parses the FullProf .sum file associated with the loaded .prf and presents structured tables of the refinement results. It is accessed by clicking the report button in the canvas toolbar.

Refinement Report

Overall profile R-factors and goodness-of-fit indicators for each diffraction pattern. Columns marked 'no bkg' correspond to R-factors reported by FullProf without the background contribution.

Pattern	Rp (%)	Rwp (%)	Rexp (%)	χ^2	Rp (no bkg)	Rwp (no bkg)	χ^2 (no bkg)	DW-stat	Nobs
1	8.980	8.800	2.740	10...	3.050	4.050	10.300	0.756	181

Copy Table 1 (TSV) Export Table 1 to Word

Table 2. Refined Unit-cell Parameters, Volumes and Densities
Lattice parameters, cell volume and density with estimated standard deviations (e.s.d.) in parentheses. PM = Profile Matching (no structural model). Fixed parameters have no e.s.d.

Pattern	Phase	Type	Sp. Gr.	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å ³)	Density (g/cm ³)
1	DyMnGe6 ...	Rietv...		5.20...	5.20...	8.15...	90.0...	90.0...	120.0...	191.5...	—

Format: refined value(e.s.d.) → e.g. 5.4312(8) means 5.4312 ± 0.0008 Å

Copy Table 2 (TSV) Export Table 2 to Word

Table 3. Phase Fractions and Crystallographic R-factors
Bragg and structure-factor R-values per phase. Phase fractions are mass percentages with e.s.d. in parentheses.

Pattern	Phase	Type	R _{Bragg} (%)	R _f (%)	Phase fraction (%)
---------	-------	------	------------------------	--------------------	--------------------

Copy all tables (TSV) Export all tables to Word (.docx) Close

Report viewer displaying the refinement results extracted from the FullProf .sum file associated with the current .prf file.

Table	Contents
Table 1 - Agreement factors (single-crystal)	RF2, RF2w, RF, χ^2 (Intens), χ^2 (global), number of reflections
Table 2 - Unit-cell parameters	a, b, c, α , β , γ , density (g/cm ³) with estimated standard deviations
Table 3 - Scale and extinction	Scale factor and extinction parameters per phase
Table 4 - Atomic positions	Fractional coordinates x, y, z, thermal B factor, occupancy and multiplicity per atom
Table 5 - Magnetic moments	Components M _x , M _y , M _z , modulus M and phase angle (when applicable)

Each table has its own buttons for:

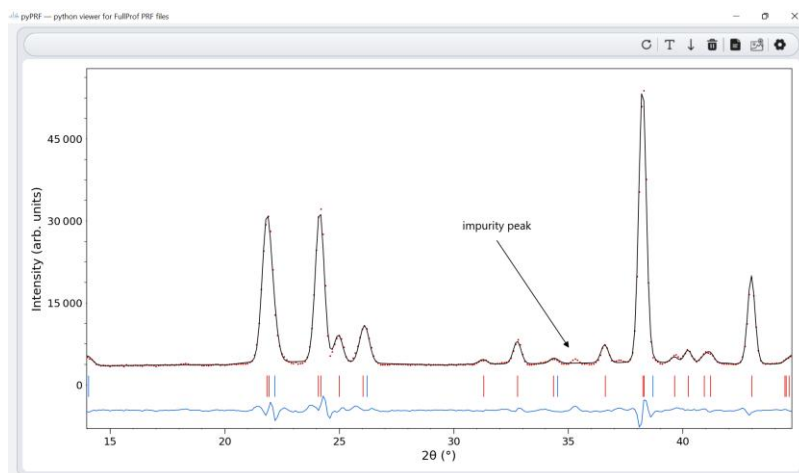
- **Copy (TSV):** copies the table to the clipboard in TSV format, ready to paste into Excel, LibreOffice Calc or any spreadsheet application.
- **Export to Word:** saves the table as a .docx document using python-docx. If this library is not installed, pyPRF shows a message and provides the installation command.

An Export all to Word button at the bottom of the dialog generates a single .docx document containing all five tables, ready for direct inclusion in publications or lab reports.

TIP: e.s.d. notation: Values are displayed in compact notation value(e.s.d.), e.g. 5.4312(8) means 5.4312 ± 0.0008 Å. Fixed (non-refined) parameters carry no e.s.d.

10.4.9 Annotation tools

pyPRF allows text labels and arrows to be added directly onto the plot. Annotations are stored per file: each .prf file maintains its own independent set of annotations.



Example of plot annotations in pyPRF, including custom text labels and arrows for highlighting relevant features of the diffraction pattern.

Text annotations

- Click the  button in the toolbar to activate text mode (the cursor changes to a crosshair).
- Click the point on the plot where you want to place the label.
- Type the text in the dialog that appears and confirm with OK.
- Annotations can be repositioned by dragging them with the mouse. Click an annotation to select it (highlighted border).
- The label style (font family, size, style normal/italic/bold, and colour) is controlled in the Annotations section of the settings panel. Style changes can be applied to all existing annotations by enabling the corresponding option.

Arrow annotations

- Click the arrow button  in the toolbar to activate arrow mode.
- Click the arrow origin point (tail) and then the destination point (head).
- Arrow colour, line width and head size are adjusted in the Annotations section of the settings panel.

Removing annotations

- Select an annotation and click the delete button () to remove only that annotation.
- If no annotation is selected, the  button removes all annotations for the current file.

10.4.10 Detailed appearance settings

Size and resolution

Controls the physical dimensions of the exported figure and the image resolution. The DPI value only affects export; it does not alter the on-screen appearance.

Parameter	Default value
Width (fig_width)	10.0 inches
Height (fig_height)	6.0 inches

DPI	300 (publication quality)
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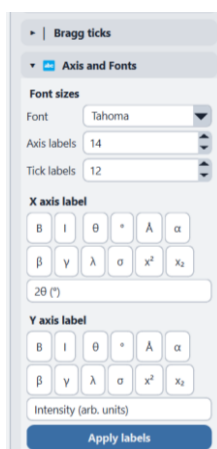
Line widths

All plot elements can be adjusted independently. A value of 0 means the base width (lw_base) is used, or lw_base × 0.85 for secondary elements.

Parameter	Description
Base	Reference line width used when individual values are 0 (default: 0.9 pt)
Observed mode	Toggle between continuous line or individual points for the observed data
Observed line / points	Line width (line mode) or marker size (points mode)
Calculated	Line width of the calculated profile
Difference	Line width of the difference curve
Background	Line width of the calculated background (visible only when enabled)

Axis labels and fonts

Axis labels accept plain text, Unicode characters and LaTeX expressions using the $\$...\$$ syntax. For example, to write 2θ (°) with a mathematical theta use $\$2\backslash\theta\$$ (°). Changes are applied by pressing the Apply button below the text field.



Configuration panel for axis labels and font settings. Users can define custom X- and Y-axis labels and insert special characters commonly used in scientific plots.

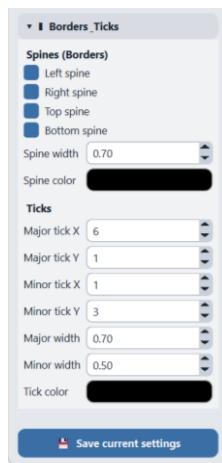
TIP: Symbol toolbar: The axis label field includes a toolbar with symbols commonly used in crystallography ($\text{\AA}$, °, α , β , γ , θ , λ ...) that can be inserted at the cursor position with a single click.

Borders and axis ticks

Controls which spines of the axes are visible and the appearance of major and minor tick marks.

Parameter	Description
Left / right / top / bottom spine	Enable or disable each spine independently

Spine width and colour	Line thickness and colour (colour picker)
Major / minor tick size	Length of major and minor ticks in points
Major / minor tick width	Thickness of ticks in points
Tick colour	Uniform colour applied to all axis ticks



Configuration panel for plot borders and tick marks. Users can control the visibility of individual spines, adjust tick density and line widths, and modify the colors of borders and ticks.

10.4.11 Figure export

The figure can be exported from the save button in the toolbar . pyPRF displays a save dialog with the available formats:

Format	Recommended use
PNG (.png)	High-resolution raster figures for reports and presentations
TIFF (.tiff)	Preferred format for many scientific journals for raster images
JPEG (.jpg)	Lossy compression; suitable for previews. pyPRF adds a white background automatically (JPEG does not support transparency)
PDF (.pdf)	Vector document; ideal for LaTeX (pdflatex, lualatex)
SVG (.svg)	Scalable vector graphic; editable in Inkscape or Illustrator
EPS (.eps)	Classic vector format; compatible with LaTeX (dvips)

If the filename typed by the user does not include an extension, pyPRF automatically appends the extension corresponding to the selected filter. The raster image resolution (PNG, TIFF, JPEG) is controlled by the DPI parameter in the Size & Resolution section.

10.4.12 Parameters and default values

All appearance parameters are defined in the DEFAULTS dictionary in main.py. They can be modified in the settings panel at runtime without editing the source code. Values changed through the interface are saved permanently via the Save current settings button and restored at each new session through QSettings.

TIP: Advanced editing: Advanced users may edit the `DEFAULTS` dictionary in `main.py` to change the startup values for a shared installation. These values have lower priority than the user-saved configuration.

The most frequently adjusted parameters are:

Parameter (key)	Default value
fig_width / fig_height	10.0 / 6.0 inches
dpi	300
lw_base	0.9 pt
obs_style	"line" (continuous line)
tick_height	1.0 (relative Bragg tick height)
bragg_shift_k	0.12 (Bragg band downward shift)
bragg_height_k	0.07 (Bragg band height)
fontsize / ticksize	14 / 12 pt
xlabel	"2 θ (°)" (auto-adapted for TOF)
ylabel	"Intensity (arb. units)"
mono_view	"stl" ($F^2_{\text{obs}} - F^2_{\text{cal}}$ vs $\sin(\theta)/\lambda$)

10.4.13 Typical workflows

Static refinement (post-processing)

1. Run FullProf to generate the .prf and .sum files.
2. Open pyPRF and load the .prf file via Add file or from PANDA.
3. Review the plot: zoom into regions of interest with the mouse wheel and inspect hkl indices by hovering over Bragg tick marks.
4. Open the refinement report (report button) to review R-factors, cell parameters and atomic positions.
5. Adjust the visual appearance in the right panel (size, line widths, fonts, etc.).
6. Add text or arrow annotations if needed.
7. Export the figure in the format required by the journal or report (PNG 300 DPI, PDF, SVG, EPS...).
8. Export the report to Word from the report viewer for direct inclusion in the manuscript.

Real-time monitoring

9. Load into pyPRF the .prf file that FullProf will update during the refinement.
10. Activate Live mode by clicking the Live button for that file in the left-panel list.
11. Launch the refinement in FullProf. The plot updates automatically with each cycle.

12. Once convergence is reached, deactivate Live mode and proceed with the export steps described above.

TIP: Use Live mode during an active FullProf refinement to monitor the fit evolving in real time. Once convergence or the maximum number of refinement cycles is reached, adjust the plot appearance using the right panel settings and export a publication-ready figure directly from pyPRF in PNG, PDF, SVG or EPS format, without any post-processing.

10.4.14 Technical code description

This section provides an overview of the internal organisation of main.py to assist with code maintenance, development, and future extensions. It is not intended to be a complete line-by-line description of the implementation. Instead, it introduces the main components, data flow, and design principles of the application, helping developers and advanced users understand how the code is structured and where specific functionalities are implemented. Readers interested in modifying or extending PANDA can use this section as a starting point before exploring the source code in greater detail.

Module structure

Block	Description
DEFAULTS	Dictionary of all appearance parameters with their default values. This is the only place that needs to be edited to change startup values for a shared installation.
parse_sum()	State machine that parses the FullProf .sum file. Extracts agreement factors, cell parameters, atomic positions, magnetic moments, scale factors and extinction parameters using regular expressions. Supports the parenthesised e.s.d. notation, e.g. 5.4312(8).
ReportDialog / MonoReportDialog	Modal dialogs displaying the structured tables of the refinement report. Each table has individual Copy TSV and Export to Word buttons, in addition to global buttons to operate on all tables at once.
parse_powder_prf()	Reads the powder .prf file line by line. Separates data rows (2 θ , Yobs, Ycal, Ydiff, Backg) from Bragg reflection lines identified by the presence of parentheses. Handles superspace groups (propagation vectors, reflection types) and multiple wavelengths.
parse_mono_prf()	Reads the single-crystal .prf file with columns $\sin(\theta)/\lambda$, Gobs, Gcal, Sigma, DIF/Sigma, h, k, l, iv.
detect_prf_type()	Detects whether a .prf file is powder or single-crystal by searching for keywords in the header ('Sintheta', 'Gobs', 'Gcal' for single-crystal; '2Theta' for powder).
RietveldCanvas	FigureCanvas subclass. Manages the full plot drawing (_draw, _draw_mono, _draw_mono_scatter methods), mouse interaction (scroll zoom, drag, right-click reset), hkl popup tooltips, and text/arrow annotations with selection and drag repositioning.
MainWindow	Main PySide6 window. Builds the three panels using QSplitter, manages the file list (QTableWidget), Live mode (QFileSystemWatcher + QTimer), the toolbar and the collapsible settings panel. Parameter changes are debounced 120 ms before triggering a redraw.

<code>launch_pyprf()</code>	Entry point for launching pyPRF from PANDA. Detects whether a <code>QApplication</code> instance already exists, reuses it, and loads the appropriate style overlay to match the parent launcher's active theme (light/dark).
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Internal data flow

The data cycle in pyPRF follows this order for each loaded file:

- `detect_prf_type()` determines whether the file is powder or single-crystal.
- `parse_powder_prf()` or `parse_mono_prf()` reads the file and returns a Python dictionary containing numpy arrays of intensities, Bragg positions, hkl indices, exclusion mask and header metadata.
- The dictionary is stored in the `MainWindow` internal list `_prf_list` together with the file path.
- When a file is selected, `RietveldCanvas.load()` receives the dictionary and the current parameters dictionary and calls `_do_redraw(full=True)`.
- `_do_redraw()` renders all elements (profile, difference curve, tick marks, excluded regions, annotations, axes, legend) onto the matplotlib canvas and calls `draw()` to refresh the display.
- Any parameter change in the right panel triggers `_param_changed()`, which updates the `_params` dictionary and starts the debounce timer. After 120 ms, `_do_redraw()` is called again preserving the current zoom level.

Annotation management

Annotations are stored as Python dictionaries in the `_annotations` list of `RietveldCanvas`, with keys for type ("text" or "arrow"), data-space coordinates and all style attributes. On each redraw, pyPRF reconstructs the matplotlib objects from these dictionaries, ensuring that annotations scale and position correctly after a zoom or parameter change.

Theme compatibility

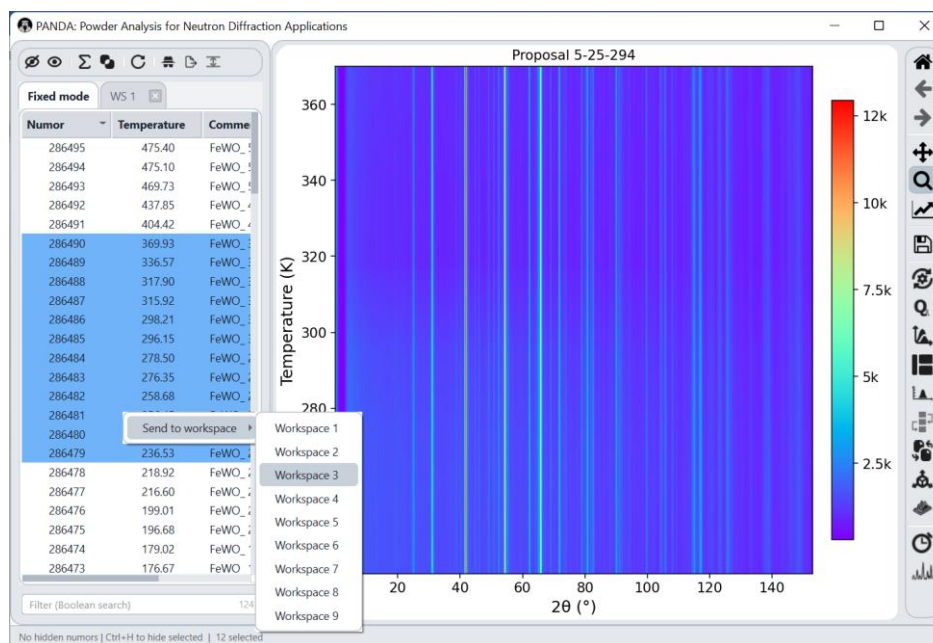
pyPRF defines its own complete set of CSS styles through the `APP_QSS` variable. All selectors are anchored to `QMainWindow` and `QDialog` to avoid conflicts with the `QApplication`-level stylesheet applied by PANDA. When launched from PANDA, pyPRF detects the active theme (light/dark) and loads a specific style overlay to maintain visual consistency with the parent window.

11. Workspaces

PANDA supports multiple independent workspaces, each with its own dataset list. Workspaces allow parallel analysis sessions without mixing datasets from different contexts.

11.1 Using Workspaces

- Tabs at the top of the left panel switch between workspaces
- Datasets can be sent to a workspace via control + right-click context menu
- Each workspace maintains its own selection, hidden state, and combined datasets
- Workspaces can be closed (datasets return to the main list)

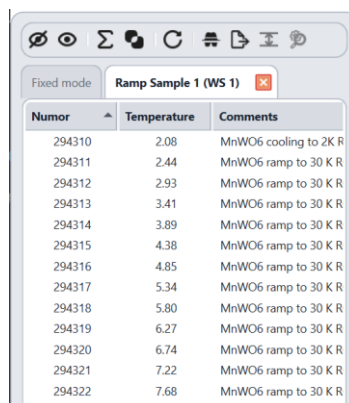


Workspace management in PANDA. Right-clicking on a selected numor opens the Send to workspace context menu, allowing the user to assign the selected datasets (here the 12 selected numors will be moved to WS3) to any of the nine available workspaces. The active workspaces appear as tabs at the top of the left panel (Fixed mode and WS 1 are currently open). Each workspace maintains its own independent dataset list, selection state, hidden numors, and combined datasets. Closing a workspace tab returns its datasets to the main list.

11.2 Renaming a Workspace

Workspace tabs are labelled *WS 1*, *WS 2*, ... by default. A workspace can be given a descriptive name so that its tab reflects the sample or the analysis it holds, while the original workspace number remains visible in brackets.

- Double-click a workspace tab to rename it, or right-click the tab and choose Rename workspace...
- Type the name in the dialog and confirm. The tab is relabeled in the form *Name (WS n)*, for example, a workspace named *Sample1* becomes *Sample1 (WS 1)*.
- The workspace number is always kept in brackets, so the origin of the datasets can still be identified at a glance in menus, dialogs and messages.



The screenshot shows the PANDA software interface. At the top, there is a toolbar with icons for various functions. Below the toolbar, there are two tabs: 'Fixed mode' and 'Ramp Sample 1 (WS 1)'. The 'Ramp Sample 1 (WS 1)' tab is active. Below the tabs, there is a table with three columns: 'Numor', 'Temperature', and 'Comments'. The table contains 13 rows of data.

Numor	Temperature	Comments
294310	2.08	MnWO6 cooling to 2K R
294311	2.44	MnWO6 ramp to 30 K R
294312	2.93	MnWO6 ramp to 30 K R
294313	3.41	MnWO6 ramp to 30 K R
294314	3.89	MnWO6 ramp to 30 K R
294315	4.38	MnWO6 ramp to 30 K R
294316	4.85	MnWO6 ramp to 30 K R
294317	5.34	MnWO6 ramp to 30 K R
294318	5.80	MnWO6 ramp to 30 K R
294319	6.27	MnWO6 ramp to 30 K R
294320	6.74	MnWO6 ramp to 30 K R
294321	7.22	MnWO6 ramp to 30 K R
294322	7.68	MnWO6 ramp to 30 K R

Example of renaming of a Workspace in PANDA. Double-clicking on a selected WS label opens the renaming window, allowing the user to modify the label of the selected WS.

The name is a label only. Renaming a workspace does not move, copy or modify any dataset: the tab still holds the same datasets, the Send to workspace menu still refers to the same workspace number, and the tab close button still closes that workspace. Only the text on the tab changes.

Removing the name restores the default label. Reopen the rename dialog, clear the text field and confirm: the tab reverts to *WS n*. A name made only of spaces is treated as empty and has the same effect.

Names are kept for the current session only. Closing a workspace tab discards its name together with its dataset list, and closing PANDA discards the names of all workspaces, as it does the workspaces themselves, which are not saved between sessions. When PANDA is restarted, workspaces are created again as *WS 1*, *WS 2*, ... and can be renamed as required.

Only workspace tabs can be renamed. The fixed dataset tabs (Fixed mode, 2θ scans, TOF, and the other scan-type tabs) do not respond to double-click or to the rename menu.

12. Understanding the Data

This section provides scientific background on the data representations, normalization options, and statistical handling used in PANDA. Understanding these concepts helps users make informed choices when configuring and interpreting results.

12.1 Monitor Normalization vs. Time Normalization

PANDA supports both monitor normalization and time normalization.

Monitor normalization compensates for fluctuations in reactor flux during acquisition and is therefore generally preferred for neutron diffraction experiments. It divides each dataset by its monitor count, ensuring that variations in beam intensity do not affect the measured relative intensities.

Time normalization divides intensities by the counting time (in seconds). This is useful for comparing measurements acquired under stable beam conditions or when monitor information is unavailable.

IMPORTANT: Monitor normalization is strongly recommended as the default for neutron diffraction experiments, as it directly corrects for beam flux variations between measurements.

12.2 2θ and Q Representations

The default diffraction axis is 2θ , expressed in degrees. This is the direct angular output of the detector position.

PANDA also supports conversion to momentum transfer Q, defined as:

$$Q = 4\pi \sin(\theta) / \lambda$$

where λ is the neutron wavelength in Ångströms.

Working in Q-space is particularly useful for comparing datasets measured with different wavelengths, or for comparing measurements from multiple instruments or experimental configurations. Peak positions in Q-space are instrument-independent and directly related to d-spacings via $Q = 2\pi/d$.

12.3 Error Propagation

When combining, averaging, or subtracting datasets, PANDA propagates statistical uncertainties automatically. Variances are accumulated during sums and scaled correctly during normalization. This ensures that exported datasets retain meaningful uncertainties for subsequent Rietveld refinement or further analysis.

For instruments with a 2D detector the uncertainty of each point of the integrated pattern is propagated from the counting statistics of the contributing detector pixels: each virtual-detector pixel carries its Poisson-propagated sigma, and these are combined over the pixels that fall in the

same 2θ channel. D16 and XtremD apply this and nothing else. D2B additionally applies an empirical-dispersion floor, which raises sigma only where the pixels of a channel scatter by more than counting statistics alone would explain.

13. Instrument-Specific Behaviour

PANDA supports four ILL instruments. This section describes instrument-specific details that affect data loading, visualization, and analysis workflows.

13.1 D20

D20 is a high-flux powder diffractometer at the ILL, typically used for rapid data acquisition and temperature-dependent studies. Datasets are collected using a large position-sensitive detector covering a wide angular range.

PANDA supports rapid visualization of D20 temperature series and live acquisition workflows. Incremental reload (Ctrl+R) is particularly useful during active experiments on D20.

13.2 D1B

D1B is a medium-resolution powder diffractometer at the ILL, commonly used for magnetic structure determination and studies requiring high sensitivity.

PANDA supports D1B NeXus files and includes fallback ASCII reading modes when required. Fixed detector scans and live monitoring workflows are fully supported.

D1B NeXus files contain both **raw detector counts** and **efficiency-corrected data**. PANDA automatically selects the appropriate dataset depending on the workflow chosen by the user. If no detector calibration file is provided, PANDA uses the efficiency-corrected data stored in the NeXus file, which have been calibrated by NOMAD. Alternatively, if a detector calibration file is supplied, PANDA reads the raw detector counts and applies the user-provided efficiency calibration during data reduction. This approach ensures full compatibility with both the standard D1B processing chain and custom detector calibrations without requiring any manual intervention.

13.3 D2B

D2B is a high-resolution powder diffractometer at the ILL, featuring a large 2D detector that allows high counting statistics. PANDA provides dedicated support for D2B including:

- Frame-by-frame viewer: browse individual detector frames from the 2D detector
- Virtual detector reconstruction: project the 2D detector onto a 1D powder pattern
- Detector re-integration: re-integrate raw 2D detector images with configurable angular integration ranges
- Re-integrate 2D toolbar action: rebuild 1D patterns from raw detector data with updated settings

13.4 XtremeD

XtremeD is a powder diffractometer optimized for extreme conditions experiments. PANDA supports XtremeD datasets with both 1D and 2D visualization modes including:

- Frame-by-frame viewer: browse individual detector frames from the 2D detector
- Virtual detector reconstruction: project the 2D detector onto a 1D powder pattern
- Detector re-integration: re-integrate raw 2D detector images with configurable angular integration ranges
- Re-integrate 2D toolbar action: rebuild 1D patterns from raw detector data with updated settings

And temperature-dependent and/or numor-dependent datasets.

13.5 D16

D16 is a monochromatic cold neutron diffractometer equipped with a large 2D detector and optimized for diffuse scattering, reciprocal-space mapping and low-dimensional systems. PANDA supports D16 datasets with both 1D and 2D visualization modes including:

- Frame-by-frame viewer: browse individual detector frames from the 2D detector
- Virtual detector reconstruction: project the 2D detector onto a 1D powder pattern
- Detector re-integration: re-integrate raw 2D detector images with configurable angular integration ranges
- Re-integrate 2D toolbar action: rebuild 1D patterns from raw detector data with updated settings
- Reciprocal-space style visualization: direct inspection of detector intensity distributions before integration
- Temperature-dependent and/or numor-dependent datasets

Unlike D2B or XtremeD, D16 datasets are often used for diffuse scattering or strongly anisotropic intensity distributions. For this reason, inspection of the raw 2D detector images is particularly important before performing conical integration into a final 1D diffraction pattern.

13.6 Other

In addition to the natively supported ILL diffractometers, PANDA includes a generic instrument mode that activates automatically when loading datasets from unrecognised or unsupported sources. This mode is intended for data collected at instruments not explicitly configured in PANDA, or for externally processed files that need to be visualised and prepared for refinement within the same workflow.

Supported input formats

To be loaded in generic mode, files must follow one of the input formats accepted by PANDA: two-column (2 θ , I) or three-column (2 θ , I, σ I) column-format ASCII files, or Malvern Panalytical

XRDML files (.xrdml). Files with non-standard delimiters or binary formats other than XRDML are not supported in this mode.

Metadata handling

Because PANDA cannot parse instrument-specific format for unrecognised sources, automatic metadata extraction is limited. Depending on the header structure of the input files, some or all of the following fields may not be populated automatically: temperature, numor, wavelength, monitor counts, and sample information. In such cases, the user is responsible for verifying and entering the relevant metadata manually before proceeding with any reduction or export operation. Incorrect or missing metadata, particularly wavelength and temperature, will affect normalization, binning, and the filename conventions used during export.

Recommended workflow

When working with generic datasets, it is advisable to inspect the imported metadata table carefully after loading and to correct any missing fields before performing combination, background subtraction, or sequential refinement export. If the wavelength is not detected automatically, it must be set explicitly, as it is required for Q-axis conversion.

14. Scientific Workflows

This section describes common scientific workflows that researchers perform with PANDA, from initial data inspection to export data for Rietveld/Lebail refinement. To improve efficiency during data analysis, PANDA also provides a set of keyboard shortcuts and mouse interactions that allow rapid dataset selection, visualization control and workspace management. The most commonly used shortcuts and interactions are summarized below.

Shortcut	Context	Action
Ctrl+H	Dataset list	Hide selected numors
Ctrl+S	Dataset list	Show all hidden numors
Ctrl+R	Dataset list	Reload folder (incremental)
Ctrl+A	Dataset list	Combine selected datasets / Select all visible numors (if no selection active)
Ctrl+D	Dataset list	Difference (subtract second from first)
Ctrl+C	Dataset list	Copy current tree selection to clipboard
Left click	Dataset list	Select / deselect a numor
Shift+Left click	Dataset list	Range selection from anchor
Right click	Dataset list	Clear all selections
Ctrl+Right click	Dataset list	Open “Send to workspace” context menu
Left click	Column header	Sort by column (ascending / descending)
Right click	Column header	Show/Hide columns context menu
Left click + drag	Canvas (plot area)	Zoom into region of interest
Right click	Canvas (inside plot)	Reset view
Right click	Canvas (outside plot)	Open colorbar context menu (show/hide colorbar)
Scroll wheel	Canvas	Apply vertical offset between 1D curves
Double click/F2	Table cell/WS labels	Edit cell/label content
F2 and Enter	Table cell (continuous rows)	Column Edit
Double click	Canvas	Activate the guide-line

14.1 Identifying Phase Transitions

Temperature-dependent phase transitions are one of the most common analysis targets in neutron powder diffraction. The recommended workflow is:

1. Load all datasets from a temperature series
2. Select all datasets (Ctrl+A to select all)
3. The view automatically switches to 2D heatmap mode
4. Examine the heatmap for sudden changes in peak position, splitting, or intensity as a function of temperature
5. Enable logarithmic color scale to reveal weak diffuse features or subtle changes
6. Use the 1D Slice panel to inspect individual temperature slices interactively

TIP: Structural or magnetic transitions often appear as peak splitting, intensity changes, or shifts in peak position. Logarithmic scale can reveal weak diffuse features that are invisible on a linear scale.

14.2 Tracking Magnetic Reflections

Magnetic scattering contributions are often weak compared to the nuclear background. The difference operation is the primary tool for isolating them:

1. Select a low-temperature dataset (below the magnetic transition)
2. Ctrl+Click to add a high-temperature reference dataset (above the transition)
3. Press Ctrl+D to compute the difference
4. The resulting difference pattern isolates the magnetic scattering contribution
5. Inspect the result for magnetic peaks not present in the high-temperature pattern

NOTE: Verify that both datasets have comparable counting statistics and normalization before interpreting weak signals in the difference pattern.

14.3 Preparing Datasets for FullProf

To obtain a high-statistics pattern suitable for Rietveld refinement with FullProf or similar codes:

1. Identify equivalent measurements collected under the same conditions
2. Select all equivalent datasets (Ctrl+Click)
3. Use Combine (Ctrl+A) to sum or average them into a single virtual dataset
4. Verify the combined pattern visually
5. Export the pattern using the Export button (choose the appropriate format for FullProf)
6. Open pyPRF via the pyPRF button to visualize FullProf PRF output files directly

14.4 Sequential Fitting

Sequential fitting extracts peak parameters across an entire temperature series automatically:

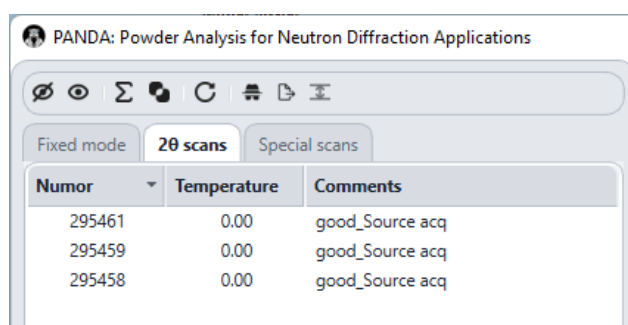
1. Select a representative dataset and activate Fit mode (Fit button in right toolbar)
2. Define the peak model by clicking on each peak position
3. Verify the fit quality on the representative dataset
4. Click Sequential Fit to propagate the model across all visible datasets
5. Export the resulting parameter table for analysis of lattice parameter or peak intensity evolution

15. Virtual Dataset Management

PANDA distinguishes between raw datasets loaded from disk and virtual datasets generated by operations such as combining or differencing. Understanding this distinction is important for avoiding errors in analysis.

Dataset type	Description
Raw dataset	Loaded directly from a NeXus (.nxs) file. The source of all experimental data.
Combined dataset	Virtual dataset generated by summing or averaging two or more raw datasets. Can be plotted and exported like a standard dataset.
Difference dataset	Virtual dataset representing the subtraction of two compatible patterns. The sign of the result depends on the order of selection. Error propagation is applied automatically.
Sequential fit output	Parameter table (not a dataset) containing peak evolution as a function of scan variable or temperature. Available for export after sequential fitting.

NOTE: User-generated datasets such as summed patterns, difference patterns, or integrations created with modified parameters (for 2D detectors) can be removed manually. To delete a virtual dataset, place the cursor over the corresponding entry in the dataset list, press **Ctrl + right click**, and then select **Delete dataset**. Only user-generated datasets can be removed; original raw datasets loaded from disk are always protected from deletion. Note that if a user-generated dataset is deleted from a specific workspace, it will also be removed from the main/general workspace from which it originates.



Automatic scan classification in PANDA. For instruments supporting multiple scan types, PANDA automatically identifies and classifies the datasets according to their acquisition mode. The different scan categories are then displayed in separate tabs, allowing the user to easily distinguish, organize and process each type of measurement independently.

15.1 Compatibility Constraints

- Combined datasets cannot be recombined with raw datasets
- Difference operations require exactly two datasets with compatible X axes
- Already-differenced datasets cannot be differenced again
- All datasets in a combine or difference operation must come from the same instrument

16. Advanced Features

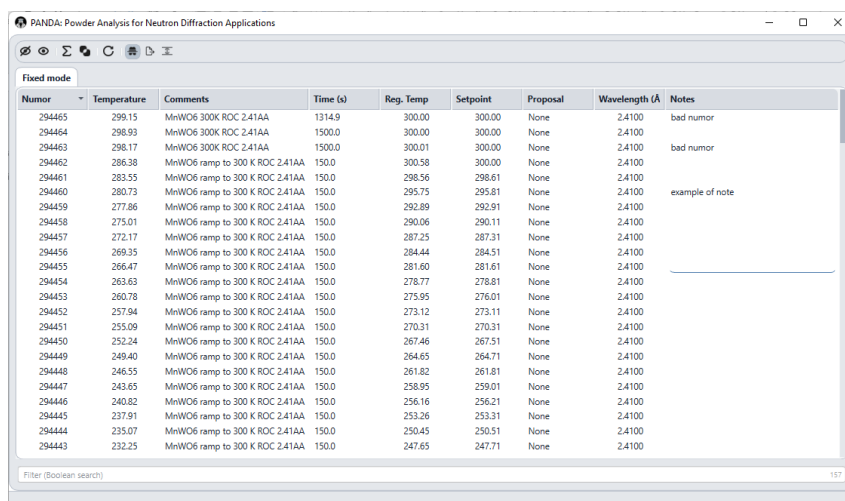
16.1 Boolean Filter

The search box at the bottom of the dataset list accepts Boolean expressions to filter numors. Examples:

- "296" — shows all numors containing "296" in any field
- "FeWO4 AND 300" — shows numors matching both terms
- "NOT hidden" — excludes hidden numors

16.2 Spy Mode

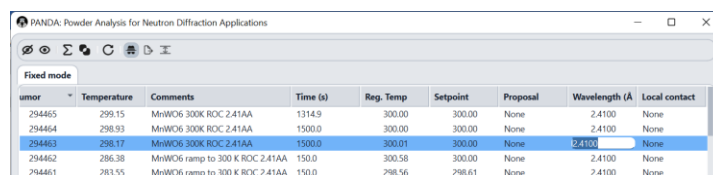
Spy mode (toolbar) maximizes the dataset list to full width and reveals all available metadata columns (instrument, scan type, monitor, wavelength, etc.). This is useful for data inspection without plotting.



The screenshot shows the PANDA application window in Spy Mode. The toolbar at the top includes icons for various actions. The main area displays a table of dataset records with the following columns: Numor, Temperature, Comments, Time (s), Reg. Temp, Setpoint, Proposal, Wavelength (Å), and Notes. The table contains 20 rows of data, with some rows highlighted. A filter bar at the bottom left shows the text "Filter (Boolean search)".

Numor	Temperature	Comments	Time (s)	Reg. Temp	Setpoint	Proposal	Wavelength (Å)	Notes
294465	299.15	MnWO6 300K ROC 2.41AA	1314.9	300.00	300.00	None	2.4100	bad numor
294464	298.93	MnWO6 300K ROC 2.41AA	1500.0	300.00	300.00	None	2.4100	
294463	298.17	MnWO6 300K ROC 2.41AA	1500.0	300.01	300.00	None	2.4100	bad numor
294462	286.38	MnWO6 ramp to 300 K ROC 2.41AA	150.0	300.58	300.00	None	2.4100	
294461	283.55	MnWO6 ramp to 300 K ROC 2.41AA	150.0	298.56	298.61	None	2.4100	
294460	280.73	MnWO6 ramp to 300 K ROC 2.41AA	150.0	295.75	295.81	None	2.4100	example of note
294459	277.86	MnWO6 ramp to 300 K ROC 2.41AA	150.0	292.89	292.91	None	2.4100	
294458	275.01	MnWO6 ramp to 300 K ROC 2.41AA	150.0	290.06	290.11	None	2.4100	
294457	272.17	MnWO6 ramp to 300 K ROC 2.41AA	150.0	287.25	287.31	None	2.4100	
294456	269.35	MnWO6 ramp to 300 K ROC 2.41AA	150.0	284.44	284.51	None	2.4100	
294455	266.47	MnWO6 ramp to 300 K ROC 2.41AA	150.0	281.60	281.61	None	2.4100	
294454	263.63	MnWO6 ramp to 300 K ROC 2.41AA	150.0	278.77	278.81	None	2.4100	
294453	260.78	MnWO6 ramp to 300 K ROC 2.41AA	150.0	275.95	276.01	None	2.4100	
294452	257.94	MnWO6 ramp to 300 K ROC 2.41AA	150.0	273.12	273.11	None	2.4100	
294451	255.09	MnWO6 ramp to 300 K ROC 2.41AA	150.0	270.31	270.31	None	2.4100	
294450	252.24	MnWO6 ramp to 300 K ROC 2.41AA	150.0	267.46	267.51	None	2.4100	
294449	249.40	MnWO6 ramp to 300 K ROC 2.41AA	150.0	264.65	264.71	None	2.4100	
294448	246.55	MnWO6 ramp to 300 K ROC 2.41AA	150.0	261.82	261.81	None	2.4100	
294447	243.65	MnWO6 ramp to 300 K ROC 2.41AA	150.0	258.95	259.01	None	2.4100	
294446	240.82	MnWO6 ramp to 300 K ROC 2.41AA	150.0	256.16	256.21	None	2.4100	
294445	237.91	MnWO6 ramp to 300 K ROC 2.41AA	150.0	253.26	253.31	None	2.4100	
294444	235.07	MnWO6 ramp to 300 K ROC 2.41AA	150.0	250.45	250.51	None	2.4100	
294443	232.25	MnWO6 ramp to 300 K ROC 2.41AA	150.0	247.65	247.71	None	2.4100	

Spy mode interface in PANDA. In this mode, the dataset list is expanded to the full window width and all available metadata columns are displayed, including numor, temperature, comments, acquisition time, scan variables, proposal number and wavelength, among other parameters. Spy mode is intended for rapid inspection, comparison and sorting of experimental metadata without loading or plotting the datasets.



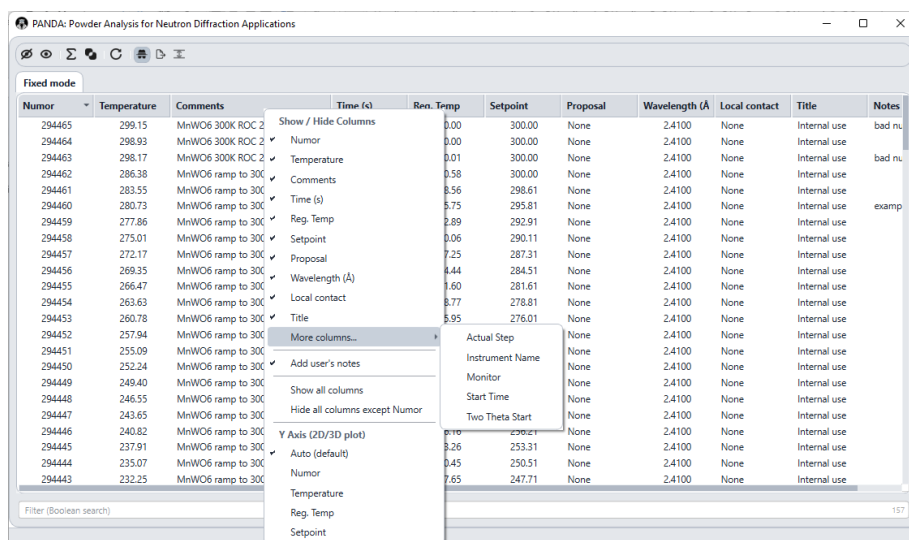
The screenshot shows the PANDA application window in Spy Mode. The toolbar at the top includes icons for various actions. The main area displays a table of dataset records with the following columns: umor, Temperature, Comments, Time (s), Reg. Temp, Setpoint, Proposal, Wavelength (Å), and Local contact. The table contains 6 rows of data, with the row for numor 294463 highlighted. A filter bar at the bottom left shows the text "Filter (Boolean search)".

umor	Temperature	Comments	Time (s)	Reg. Temp	Setpoint	Proposal	Wavelength (Å)	Local contact
294465	299.15	MnWO6 300K ROC 2.41AA	1314.9	300.00	300.00	None	2.4100	None
294464	298.93	MnWO6 300K ROC 2.41AA	1500.0	300.00	300.00	None	2.4100	None
294463	298.17	MnWO6 300K ROC 2.41AA	1500.0	300.01	300.00	None	2.4100	None
294462	286.38	MnWO6 ramp to 300 K ROC 2.41AA	150.0	300.58	300.00	None	2.4100	None
294461	283.55	MnWO6 ramp to 300 K ROC 2.41AA	150.0	298.56	298.61	None	2.4100	None

Most metadata fields can be edited directly either by double-clicking on a cell or by pressing F2 after selecting it. The numor column remains read-only. User modifications are stored in memory during the session and are automatically propagated to subsequent plotting, export, and dataset combination operations. Edits are preserved when refreshing the trees using Ctrl+R or the refresh button in the action panel.

16.3 Extra Columns

Right-clicking the column header opens a menu to add or remove optional metadata columns from the dataset list. Available fields depend on the data stored in the NeXus files.

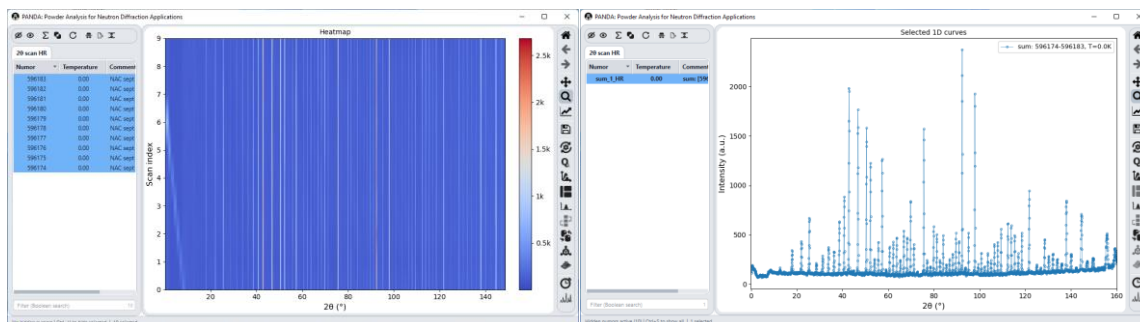


Context menu for managing metadata columns in Spy mode. Right-clicking on the dataset header opens a configurable menu that allows optional metadata fields to be added or removed from the dataset list. The available columns depend on the information stored in the NeXus files and may include experimental parameters, instrument metadata and user-defined fields (Notes).

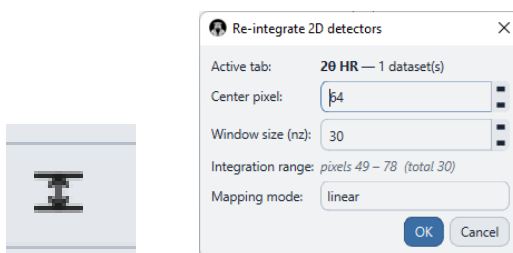
16.4 2D Detector

For D2B, D16 and XtremD instruments equipped with a 2D detector, PANDA provides additional views:

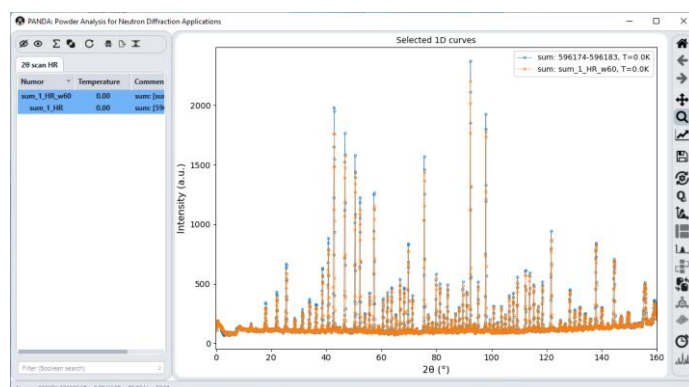
- Frame-by-frame viewer: browse individual detector frames
- Virtual detector view: project the 2D detector onto a 1D pattern



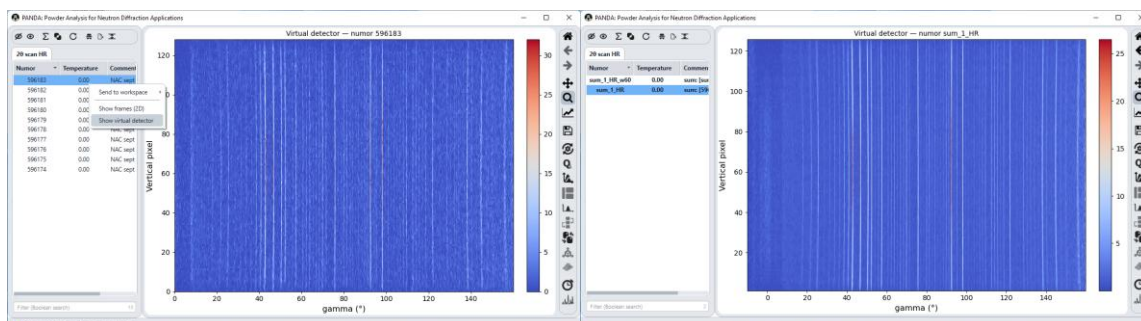
(Left) View of the 2D representation of the individual scans loaded from the experiment. Each horizontal line corresponds to one D2B scan composed of 25 detector frames acquired with successive angular offsets of 0.05° . Only the common 2θ angular range shared by all scans is displayed in the heatmap representation. (Right) Integrated 1D diffraction pattern obtained after summing the 10 individual scans shown in the left figure. The final pattern corresponds to the conical integration of the 2D virtual detector, providing the final 1D diffraction profile. The integration region uses the default detector limits defined in the startup configuration window, although these parameters can be modified interactively using the last icon in the right-side action toolbar.



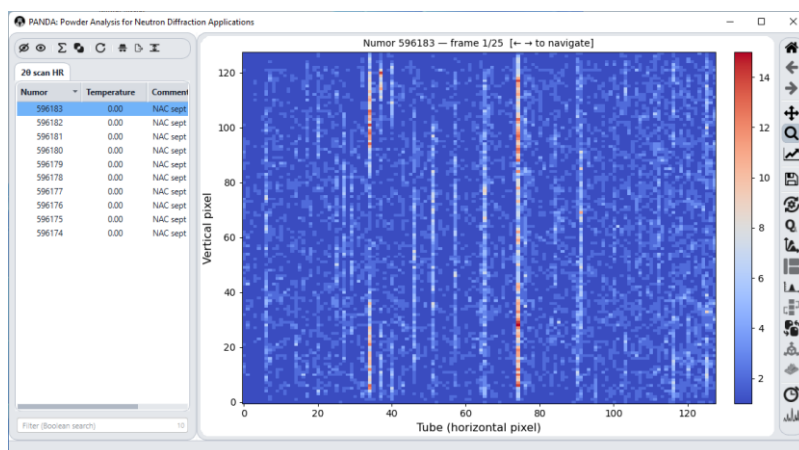
Re-integrate 2D detectors dialog accessible from the action toolbar. This window allows the user to redefine the detector integration region and the mapping mode used to reconstruct the virtual detector from the individual detector frames. The mapping mode controls how the intensity from each detector tube is projected onto the final common 2θ grid (e.g. nearest, linear or Gaussian interpolation), directly influencing the smoothness and resolution of the reconstructed 1D diffraction pattern.



If a new integration is generated, the resulting dataset will appear in the dataset list using the original dataset name followed by the suffix `_W`, where `W` corresponds to the selected integration window width.



Comparison between the virtual detector reconstructed from a single D2B scan (left) and the virtual detector obtained after combining multiple scans (right). In PANDA, the virtual detector is first reconstructed from the individual detector frames acquired at different angular offsets, generating a continuous 2D detector representation. The final 1D diffraction pattern is then obtained through conical integration of this virtual detector. Combining several scans improves the angular coverage and counting statistics of the reconstructed detector prior to the integration step.



Frame-by-frame visualization mode for a D2B. This mode can be accessed by pressing Ctrl + right click on a dataset and selecting Show frames (2D). The displayed image corresponds to an individual detector frame from the selected scan, represented as detector tube versus vertical pixel position. Navigation through the different detector frames is performed interactively using the left/right arrow keys of the keyboard.

NOTE: When working with instruments equipped with 2D detectors, PANDA automatically reconstructs the virtual detectors and performs the corresponding conical integrations before displaying the final 1D diffraction pattern. As a result, importing a large number of datasets may require significant processing time. In addition, when the data are accessed through a network connection, the loading time can increase considerably due to network latency and data transfer overhead.

17. Performance & Large Datasets

Very large temperature series may require careful management of memory and visualization settings to maintain responsiveness.

17.1 General Recommendations

- Use incremental reload rather than full reload during live acquisition
- Limit the number of simultaneously visible datasets (configure Max 1D curves in the Configuration window)
- Avoid unnecessary redraws during live acquisition
- Close unused workspaces to free memory

17.2 Heatmap Performance

- Logarithmic color scales may increase rendering time for large heatmaps
- Reduce the number of Temperature interpolation points in the Configuration window if heatmap rendering is slow
- Consider disabling logarithmic visualization for very large datasets during initial exploration

17.3 Advanced fine-tune

Advanced users can fine-tune PANDA's behaviour by manually editing `user_config.py` with a text editor. Beyond the standard settings managed through the Configuration window, the following internal parameters are available directly in the file:

Parameter	Example value	Description
CMAP	"rainbow", "viridis"...	Colormap for 2D heatmap
SPIKE_FACTOR	5.0 (0 = disabled)	D20 spike rejection threshold
MOTOR_JITTER	0.004 (degrees 2 θ)	D20 encoder noise floor
FONT_SIZE_*	12 / 14 / 12	Title, label, tick font sizes
TEMPERATURE	"temperature"	NeXus temperature field to read
WAVELENGTH	None or 2.52 (Å)	Override NeXus wavelength
THEME	"auto", "light", "dark"	UI colour theme
ATOL_2THETA	0.004 (degrees)	2 θ axis matching tolerance

These parameters are marked "do not edit" in the file but can be safely modified by advanced users.

If a `user_config.py` file is present in the project folder, the parameters defined in this file take precedence over the **default values** loaded by PANDA. This allows users to customize the behaviour of the program on a per-project basis without modifying the internal default configuration files.

18. Architecture Overview

This section provides a brief description of the main software modules that constitute PANDA, intended for advanced users who need to understand or extend the application.

Module	Role
io_nexus.py	Handles reading of NeXus HDF5 files. Parses instrument-specific data paths, extracts diffraction patterns, metadata, and monitor information. Includes ASCII fallback logic for D1B.
processing.py	Implements dataset operations: normalization, binning, combining, differencing, error propagation, and peak fitting. All virtual dataset computations are performed here.
visualization modules	Responsible for 1D pattern plotting, 2D heatmap rendering, 3D surface and waterfall views, and the interactive slice panel.
user_config.py	Stores all user configuration parameters. Read at startup and updated on each configuration change. Can be edited manually for batch configuration.

18.1 Processing Pipeline

The typical data processing pipeline in PANDA follows this sequence:

1. NeXus file read by io_nexus.py
2. Detector calibration applied (if a calibration file is configured)
3. Normalization applied (monitor or time)
4. Binning applied (if enabled)
5. Baseline subtracted (if a baseline file is configured)
6. Dataset made available for visualization and further operations

19. user_config.py Reference

The `user_config.py` file stores all user preferences and is automatically updated by the Configuration window. It can also be edited manually with any text editor for batch setup or advanced configuration.

19.1 Example Settings

Parameter	Example value / description
instrument	"D20" — instrument name string
project_folder	"/data/proposal_1234" — path to project folder
data_folder	"/data/proposal_1234/raw" — path to NeXus files
file_extension	".nxs" — file extension to scan for
two_theta_offset	0.0 — angular offset in degrees
scale_factor	1.0 — global intensity scale factor
normalize_by_monitor	True — enable monitor normalization
normalize_by_duration	False — disable time normalization
binning	True — enable angular rebinning
temperature_interp_points	200 — Y-axis interpolation for heatmap
max_1d_curves	5 — maximum 1D overlays before switching to heatmap
wavelength_override	1.594 — override instrument wavelength in Å (if needed)
baseline_file	"/data/proposal_1234/raw/baseline.nxs" — background reference
baseline_temperature	None — disable temperature-based baseline selection

TIP: The `wavelength_override` parameter is useful when the wavelength stored in the NeXus file is incorrect or when comparing datasets from different experimental configurations.

20. Troubleshooting

Problem	Solution
No files appear in the dataset list	Verify that the configured data folder contains supported NeXus (.nxs) files and that the Instrument setting matches the dataset type. Check the File extension setting.
Difference operation is disabled	The Difference operation requires exactly two compatible datasets with matching X axes to be selected. Verify the selection and ensure binning is enabled if the datasets have slightly different detector grids.
Heatmap is empty	Heatmaps require multiple datasets sharing a common scan variable such as temperature. Ensure that more than one dataset is selected and that temperature metadata is available.
Slow visualization	Reduce the number of simultaneously plotted datasets. Disable logarithmic visualization for very large datasets. Reduce Temperature interpolation points in the Configuration window.
Missing metadata columns	Some metadata fields depend on data stored in the NeXus files. Not all instruments write all fields. Use Spy mode to see which columns are available for your dataset.
Combine operation disabled	All selected datasets must come from the same instrument and scan type. Combined datasets cannot be recombined with raw datasets.
Incorrect peak positions after fitting	Check the 2θ offset setting in the Configuration window. A non-zero offset shifts all peak positions by a fixed amount.
NeXus files not recognized	Ensure the Instrument setting matches the actual instrument that produced the data. D20, D1B, D2B, and XtremD each have different NeXus path conventions.

21. Best Practices

Following these recommendations will help ensure reliable, reproducible, and publication-ready results with PANDA.

21.1 Normalization

- Always use monitor normalization for neutron diffraction experiments unless there is a specific reason to avoid it
- Only switch to time normalization when monitor information is unavailable or unreliable
- Verify that normalization is consistent across all datasets before combining or differencing

21.2 Combining Datasets

- Only combine measurements collected under equivalent experimental conditions (same temperature, same phase, same sample)
- Verify visually that the individual patterns are consistent before combining
- Document which numors were combined for reproducibility

21.3 Subtraction Workflows

- Use subtraction carefully and verify background compatibility before interpreting weak signals
- Ensure both datasets have similar counting statistics to avoid artifacts in the difference pattern
- Check the sign convention: the second selected dataset is subtracted from the first

21.4 Exporting Publication-Quality Figures

- Use vector export formats (PDF or SVG) whenever possible for publication figures
- PNG is suitable for presentations and reports but may show pixelation at high magnification
- For heatmaps, choose a color scale appropriate for the data range to avoid obscuring important features

21.5 Data Management

- Use workspaces to separate parallel analysis sessions
- Save the dataset log (Save Log toolbar action) to document your analysis session
- Use the Boolean filter to quickly locate specific numors in large datasets

- Keep the Configuration window settings consistent within a project to ensure reproducibility

Appendix A — Glossary

This glossary defines key terms, abbreviations and technical concepts used throughout this manual. Terms are listed in alphabetical order.

Term	Definition
2θ	The total scattering angle in powder diffraction, measured in degrees. It is the angle between the transmitted (direct) beam and the diffracted beam. All ILL powder diffractometers record intensity as a function of 2θ, which is the default diffraction axis in PANDA.
2θ offset	A rigid angular correction (in degrees) applied to all 2θ values in a dataset. It corrects a systematic zero-point error in the detector position: $2\theta_{\text{corrected}} = 2\theta_{\text{raw}} + \text{offset}$. Set in the PANDA Configuration window; default value is 0.0.
Baseline	A reference diffraction pattern (e.g. measured from an empty sample environment or from the sample above a transition temperature) that is automatically subtracted from all loaded datasets when a baseline file is configured. The result isolates the contribution of the sample above the background.
Binning	Rebinning of raw diffraction data onto a regular 2θ (or Q) grid with a fixed step size. Required when combining or differencing datasets whose native detector grids differ slightly (e.g. due to small shifts in detector position). Controlled in the PANDA Configuration window.
Block difference	Batch version of the difference operation: pressing Ctrl+D with more than two datasets selected opens a dialog to choose a baseline pattern, which is then subtracted from every other selected numor of the same scan type. One difference dataset per numor is created (named numor-baseline) and gathered in a new Workspace, each one keeping the temperature of its source numor so the subtracted signal can be plotted as a ramp in 2D and 3D.
Boolean filter	A text search box at the bottom of the PANDA dataset list that accepts logical expressions (AND, OR, NOT) to filter visible numors by any metadata field. Examples: '296' shows all numors containing '296'; 'FeWO4 AND 300' shows only numors matching both terms.
Bragg peak	A sharp intensity maximum in a diffraction pattern occurring when the Bragg condition is satisfied ($n\lambda = 2d \sin\theta$) for a set of crystallographic planes (hkl). Peak positions encode the crystal structure; peak intensities encode atomic positions and scattering lengths.
Calibration file	An instrument-specific file (e.g. .241 format for D20) containing per-pixel efficiency correction factors for the detector bank. When configured, PANDA applies these corrections during data loading to equalise the sensitivity of individual detector channels.
Combined dataset	A Virtual Dataset produced by summing or averaging two or more raw datasets (Ctrl+A). Useful for building a high-statistics pattern from repeated measurements under identical conditions.
d-spacing	Interplanar spacing in a crystal lattice (units: Å), related to the scattering angle by Bragg's law: $\lambda = 2d \sin(\theta)$, and to momentum transfer by $d = 2\pi / Q$.
D16	Monochromatic cold neutron diffractometer at the ILL, equipped with a large 2D detector and optimised for diffuse scattering, reciprocal-space mapping and low-dimensional systems.
D1B	Medium-resolution powder diffractometer at the ILL, typically used for magnetic structure determination and for temperature-dependent studies requiring high neutron sensitivity.

D20	High-flux powder diffractometer at the ILL, designed for rapid data acquisition and temperature-dependent studies. It features a large position-sensitive detector bank covering a wide angular range ($\approx 153^\circ$).
D2B	High-resolution powder diffractometer at the ILL. It uses a large 2D detector providing high counting statistics and supports frame-by-frame inspection of individual detector frames together with virtual detector reconstruction.
Difference dataset	A Virtual Dataset produced by subtracting one diffraction pattern from another (Ctrl+D). The second selected dataset is subtracted from the first. Error propagation is applied automatically. Used to isolate magnetic scattering or to remove a background pattern.
Error propagation	Calculation of statistical uncertainties through arithmetic operations. When PANDA combines, averages or subtracts datasets, it accumulates variances correctly (quadrature addition for sums/differences, quadrature division for averages) so that exported patterns retain meaningful σ values for subsequent Rietveld refinement.
FullProf .sum file	Summary text file generated by FullProf alongside the PRF file. It contains the refinement agreement factors (R-factors, χ^2), refined cell parameters, atomic positions, magnetic moments and scale factors. The pyPRF report viewer parses this file and presents its contents as structured tables.
GSAS .dat	ASCII data file format used by the GSAS and GSAS-II Rietveld codes for time-of-flight powder diffraction patterns (Instrument Parameter Set 12). PANDA can import GSAS .dat files in generic instrument mode and, when the calibration constants Dtt1, Dtt2 and Zero are available, convert the TOF axis to d-spacing and Q.
HDF5	Hierarchical Data Format version 5. A portable, self-describing binary file format widely used in science for storing large structured datasets. NeXus files are built on HDF5.
Heatmap	Two-dimensional colour map representing diffraction intensity as a function of the scattering coordinate (2θ or Q) on the horizontal axis and a scan variable (typically temperature) on the vertical axis. Generated automatically when several datasets are selected simultaneously in PANDA. Enables rapid visual identification of phase transitions and peak evolution.
Hover Preview	Temporary 1D diffraction pattern displayed in a floating overlay when the mouse cursor is placed over a dataset row in the PANDA dataset list, without needing to select (plot) it permanently. Allows rapid visual inspection of individual datasets in a long series.
ILL	Institut Laue-Langevin. International neutron science facility in Grenoble, France, operating one of the highest-flux steady-state research reactors in the world and providing beams for neutron scattering experiments.
Incremental reload	Dataset loading mode (Ctrl+R or toolbar button) that adds only newly detected NeXus files to the dataset list without resetting the current session state, selections or hidden numbers. Essential during live experiments to monitor incoming data in real time.
io_nexus.py	PANDA software module responsible for reading NeXus HDF5 files. Handles instrument-specific data path conventions, extracts diffraction patterns, metadata (temperature, wavelength, monitor counts, etc.) and includes ASCII fallback reading logic for D1B data.
Le Bail fit	A pattern decomposition method in which peak intensities are extracted from a diffraction pattern without a structural model, using only the peak positions implied by the unit-cell parameters. Useful for indexing new phases and for validating cell parameters before full Rietveld refinement.
Live Mode	pyPRF feature that monitors a PRF file on disk using the operating system's file watcher (QFileSystemWatcher) and automatically reloads and redraws the plot

	whenever FullProf updates the file. Allows a refinement to be observed in real time without manual intervention.
Magnetic scattering	Neutron scattering arising from the interaction of the neutron magnetic moment with unpaired electron spins in the sample. It produces additional diffraction peaks (magnetic reflections) or modifies nuclear peak intensities. Isolated by computing the difference pattern above and below a magnetic phase transition.
Monitor	A low-efficiency neutron detector placed upstream of the sample that measures the incident beam flux continuously during an acquisition. Dividing measured intensities by the monitor count (monitor normalisation) removes the effect of beam-flux variations between datasets.
NeXus	An international open standard for scientific data storage, based on HDF5 (Hierarchical Data Format version 5). All ILL instruments write their raw experimental data as NeXus (.nxs) files, which PANDA reads natively.
NeXus path	The internal slash-separated address inside a NeXus HDF5 file that locates a specific dataset or metadata field (e.g. /entry/instrument/detector/data). Different ILL instruments use different internal path conventions, which PANDA resolves automatically based on the selected instrument.
Normalization	Scaling operation applied to raw diffraction counts to remove systematic instrumental effects. PANDA supports two modes: (1) monitor normalisation, which divides by the incident beam flux monitor count; (2) time normalisation, which divides by the acquisition duration. Monitor normalisation is recommended for neutron diffraction experiments whenever monitor data are available.
Numor	Unique sequential experiment number automatically assigned by the ILL instrument control system to each data acquisition run. Each NeXus file corresponds to exactly one numor. Numors are the primary identifier used throughout the PANDA interface.
PANDA	Powder Analysis for Neutron Diffraction Applications. Scientific data browser and analysis tool for neutron powder diffraction experiments at the ILL. Supports loading, visualising, combining and exporting datasets from instruments D20, D1B, D2B, D16 and XtremeD, as well as generic ASCII and XRDML files.
Phase transition	A change in the crystal structure, magnetic ordering or electronic state of a material driven by an external parameter (temperature, pressure, field). In powder diffraction, transitions manifest as sudden changes in peak positions, intensities, multiplicities or the appearance/disappearance of peaks. Identified in PANDA from discontinuities or gradual changes in the 2D heatmap.
PRF file	Output file produced by FullProf after a Rietveld or Le Bail refinement. It contains the observed, calculated and difference diffraction profiles and is the primary input for the pyPRF viewer integrated in PANDA.
processing.py	PANDA software module implementing all dataset operations: monitor and time normalisation, angular binning, dataset combination, difference calculation, error propagation and peak fitting. All virtual dataset computations are performed by this module.
pyPRF	Interactive viewer for FullProf PRF output files, integrated in PANDA through a toolbar button. Provides real-time visualisation of the Rietveld fit (observed, calculated and difference profiles, Bragg tick marks), a Live mode for monitoring ongoing refinements, text and arrow annotation tools, a structured refinement report viewer, and publication-quality figure export (PNG, PDF, SVG, EPS, TIFF).
Q	Momentum transfer, also called scattering vector magnitude, defined as $Q = 4\pi \sin(\theta) / \lambda$ and expressed in $\text{\AA}^{-1}$. Q is wavelength-independent, making it the preferred axis for comparing data from different instruments or energies. PANDA converts 2θ to Q using the neutron wavelength stored in the NeXus file.
Rietveld Refinement	Full-pattern fitting method in which a structural model is iteratively adjusted to reproduce the observed diffraction profile. Yields refined cell parameters, atomic coordinates, thermal factors and site occupancies. Implemented in codes such as

	FullProf, GSAS and TOPAS; PANDA exports data in formats compatible with these programs.
Scale factor	A global multiplicative factor applied to all dataset intensities in PANDA. Used to rescale raw counts to match the absolute scale expected by Rietveld refinement codes, or to normalise data from different experimental runs to a common reference intensity.
Sequential fitting	PANDA mode that propagates a peak-fitting model across an entire temperature or numor series automatically. Produces a parameter table showing peak position, width and integrated intensity as a function of the scan variable. Useful for tracking lattice-parameter evolution through a phase transition.
Slice Panel	A secondary plot panel activated below the 2D heatmap in PANDA that displays in real time the 1D diffraction pattern for the row (temperature) under the mouse cursor. The panel updates continuously as the cursor moves, providing interactive inspection of any slice through the heatmap without changing the main selection.
Spy Mode	PANDA interface mode (accessible from the toolbar) in which the dataset list is expanded to the full window width and all available metadata columns are shown. Intended for rapid inspection, sorting and editing of experimental metadata without plotting datasets.
TOF	Time-of-flight. A neutron diffraction technique in which the diffraction coordinate is the neutron travel time (microseconds) from the source to the detector rather than scattering angle. TOF diffractometers use a pulsed neutron source and a wide range of neutron energies simultaneously. PANDA supports TOF data via GSAS .dat files.
user_config.py	Python configuration file maintained automatically by PANDA in the project folder. It stores all user preferences (instrument, folder paths, normalisation mode, binning, wavelength, etc.) and is restored at every startup. Advanced users can edit it manually with a text editor for batch configuration or per-project customisation.
Virtual Dataset	Any dataset generated inside PANDA by an operation (combine, difference, 2D-detector re-integration) rather than loaded directly from a NeXus file. Virtual datasets can be plotted and exported like raw datasets, but cannot be recombined with raw datasets and cannot be differenced a second time.
Virtual detector	A reconstructed 2D detector image assembled by PANDA from individual detector frames acquired at successive angular offsets (D2B, D16, XtremeD). The virtual detector provides a continuous angular coverage that can then be integrated conically into a final 1D powder diffraction pattern.
Wavelength override	A user-defined neutron wavelength value (in Å) that replaces the value stored in the NeXus file. Useful when the instrument wavelength was not written correctly to the file, or when comparing datasets recorded with slightly different monochromator settings.
Workspace	A named, independent session context in PANDA that maintains its own dataset list and selection state. Multiple workspaces allow parallel analysis threads to be kept separate within a single PANDA session.
XRDML	XML-based file format produced by Malvern Panalytical X-ray diffractometers (.xdml extension). PANDA can import and visualise XRDML files in generic instrument mode.
XtremeD	Powder diffractometer at the ILL optimised for extreme-conditions experiments (high pressure, low temperature). It is equipped with a 2D detector and PANDA provides frame-by-frame viewing and virtual detector reconstruction for its data.